

SEARCHING

Requester's Full Name: Cecilia J. Jones

Art Unit: 1634

Location (Bldg/Room): 2455 (Mailbox 1)

Serial Number: 70545-743

Results Format Preferred (circle): PAPER: ☒ DIGITAL: ☐

To ensure our information quality, please attach a copy of the cover sheet, index, and abstract or fill out the following:

Title of Invention: See Bib Data Sheet

Inventors (please provide full names):

Excluded Priority Date:

Let's try you:

[illegible]

\*Per Sequence Searching Only\* Please do not include any patient information (or any other identifying information) in the sequence.

See claims attached. Please do structure search and inventor name(s) search. Display results to show identification of source, and P.N.<sup>2</sup>, compound name and structure of identified compounds. Please do a CAS Reax search, specifying the starting materials over a product with the hydrazide substructure and a Lewis Acid in the reaction. See previous search.

Please call just a day ahead.

STAFF USE ONLY

$$\overline{\mathbf{K}}_n \mathbf{y}_n^* \mathbf{v} \in L^2(\Omega; \mathbb{R}^N)$$

Y authors not over where possible

Search: \_\_\_\_\_

H.A. Poyoung et al. (Eds.)

5/16/02

Средний балл: \_\_\_\_\_

2.  $\mathcal{F}(\mathcal{C})$  is a  $\mathcal{C}$ -category.

Question \_\_\_\_\_ Looking for \_\_\_\_\_

File type location: \_\_\_\_\_

3. **ALPHABETICALLY**

**Keywords:** *work, work-life balance, well-being, health, stress, burnout, job satisfaction, organizational commitment, turnover, organizational citizenship behavior, organizational performance*

Deutscher Fachschriften-Verlag

**Flores, Alex**

0.030 30 30.00 60 60.00 120 120.00

Date Completed: \_\_\_\_\_

L'Espresso | 25

See also 61453

Sign on File &amp; Review Date:

Phyllis:

Chlorine 35.453

በዚህ ስራ ላይ ለሚሳተፉት ሰራተኛው ስም፡ \_\_\_\_\_

訂正:

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=> file registry
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FILE 'REGISTRY' ENTERED AT 10:17:11 ON 17 OCT 2008

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10/595943

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STRUCTURE FILE UPDATES: 15 OCT 2008 HIGHEST RN 1061881-29-5  
DICTIONARY FILE UPDATES: 15 OCT 2008 HIGHEST RN 1061881-29-5

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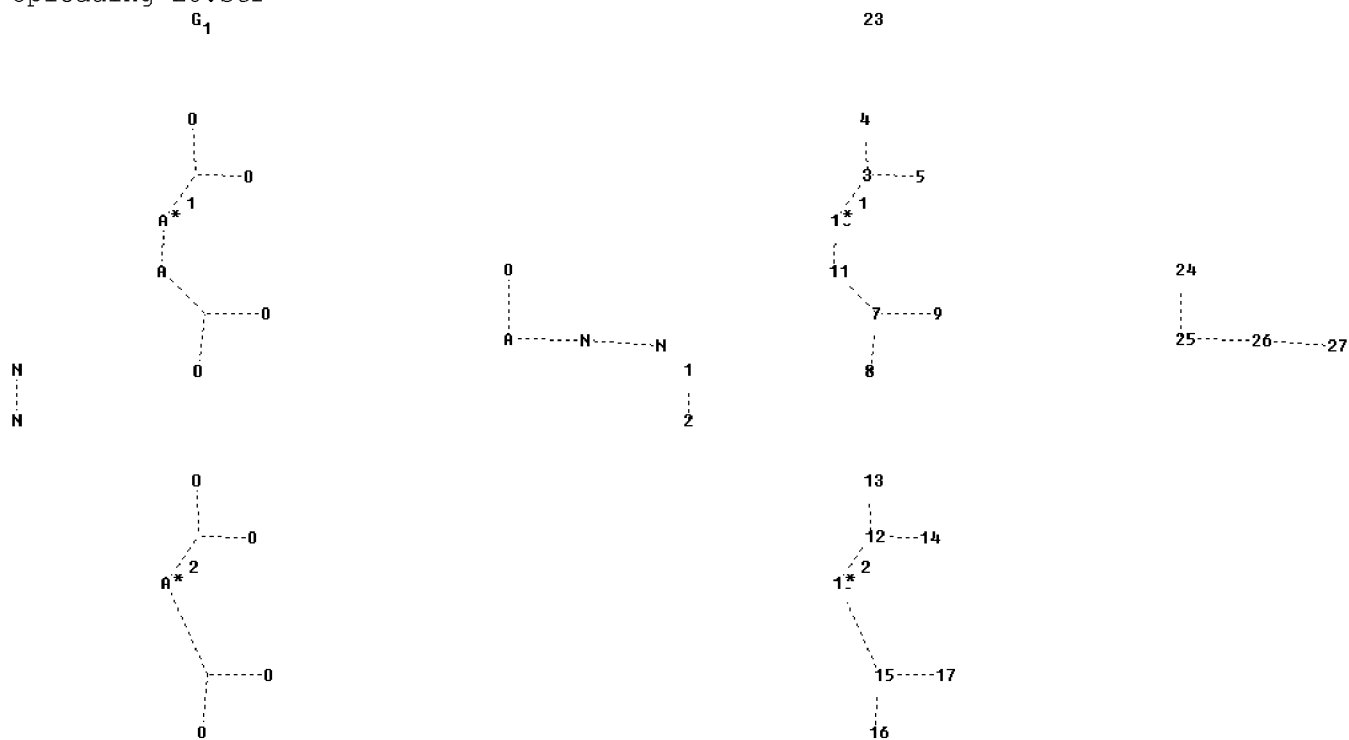
TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

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<http://www.cas.org/support/stngen/stdoc/properties.html>

Uploading L6.str



chain nodes :

3 4 5 7 8 9 12 13 14 15 16 17 23 24

ring/chain nodes :

1 2 10 11 18 25 26 27

chain bonds :

3-4 3-5 3-10 7-8 7-9 7-11 12-13 12-14 12-18 15-16 15-17 15-18 24-25

ring/chain bonds :

1-2 10-11 25-26 26-27

exact/norm bonds :

1-2 3-4 3-5 3-10 7-8 7-9 7-11 10-11 12-13 12-14 12-18 15-16 15-17 15-18

24-25 25-26 26-27

10/595943

G1:[\*1],[\*2]

Connectivity :

3:3 E exact RC ring/chain 4:1 E exact RC ring/chain 5:1 E exact RC ring/chain  
7:3 E exact RC ring/chain 8:1 E exact RC ring/chain 9:1 E exact RC ring/chain  
12:3 E exact RC ring/chain  
13:1 E exact RC ring/chain 14:1 E exact RC ring/chain 15:3 E exact RC ring/chain  
16:1  
E exact RC ring/chain 17:1 E exact RC ring/chain 24:1 E exact RC ring/chain

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
23:CLASS 24:CLASS

25:CLASS 26:CLASS 27:CLASS

fragments assigned product role:

containing 24

fragments assigned reactant/reagent role:

containing 1

containing 23

=> file caplus

FILE 'CAPLUS' ENTERED AT 10:17:14 ON 17 OCT 2008

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FILE COVERS 1907 - 17 Oct 2008 VOL 149 ISS 17

FILE LAST UPDATED: 16 Oct 2008 (20081016/ED)

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<http://www.cas.org/legal/infopolicy.html>

'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> d stat que L85

L73	643	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	LOPES C?/AU
L74	331	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	LOPES R?/AU
L75	368	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	CARDOSO J?/AU
L76	2399	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	SILVA J?/AU OR DA SILVA J?/AU OR DASILVA J?/AU
L77	1104	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	FERREIRA L?/AU
L78	28	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	L73 AND (L74 OR L75 OR L76 OR

10/595943

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          L77)
L79      8 SEA FILE=CAPLUS ABB=ON  PLU=ON  L74 AND (L75 OR L76 OR L77)
L80      2 SEA FILE=CAPLUS ABB=ON  PLU=ON  L75 AND (L76 OR L77)
L81     16 SEA FILE=CAPLUS ABB=ON  PLU=ON  L76 AND L77
L82      8 SEA FILE=CAPLUS ABB=ON  PLU=ON  L78 AND (L79 OR L80 OR L81)
L83      0 SEA FILE=CAPLUS ABB=ON  PLU=ON  L79 AND (L80 OR L81)
L84      0 SEA FILE=CAPLUS ABB=ON  PLU=ON  L80 AND L81
L85      8 SEA FILE=CAPLUS ABB=ON  PLU=ON  (L82 OR L83 OR L84)
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=> d stat que L87
L6      STR
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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

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L8      446 SEA FILE=CASREACT SSS FUL L6 ( 4732 REACTIONS)
L73     643 SEA FILE=CAPLUS ABB=ON  PLU=ON  LOPES C?/AU
L74     331 SEA FILE=CAPLUS ABB=ON  PLU=ON  LOPES R?/AU
L75     368 SEA FILE=CAPLUS ABB=ON  PLU=ON  CARDOSO J?/AU
L76    2399 SEA FILE=CAPLUS ABB=ON  PLU=ON  SILVA J?/AU OR DA SILVA J?/AU
          OR DASILVA J?/AU
L77    1104 SEA FILE=CAPLUS ABB=ON  PLU=ON  FERREIRA L?/AU
L86     446 SEA FILE=CAPLUS ABB=ON  PLU=ON  L8
L87      3 SEA FILE=CAPLUS ABB=ON  PLU=ON  L86 AND (L73 OR L74 OR L75 OR
          L76 OR L77)
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=> file medline embase biosis wpix
FILE 'MEDLINE' ENTERED AT 10:17:32 ON 17 OCT 2008
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FILE 'EMBASE' ENTERED AT 10:17:32 ON 17 OCT 2008
Copyright (c) 2008 Elsevier B.V. All rights reserved.
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FILE 'BIOSIS' ENTERED AT 10:17:32 ON 17 OCT 2008
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FILE 'WPIX' ENTERED AT 10:17:32 ON 17 OCT 2008
COPYRIGHT (C) 2008 THOMSON REUTERS
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=> s L85
L88      4 L85
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=> file zcaplus
FILE 'ZCAPLUS' ENTERED AT 10:17:43 ON 17 OCT 2008
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FILE COVERS 1907 - 17 Oct 2008 VOL 149 ISS 17  
FILE LAST UPDATED: 16 Oct 2008 (20081016/ED)

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=> file caplus

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FILE COVERS 1907 - 17 Oct 2008 VOL 149 ISS 17  
FILE LAST UPDATED: 16 Oct 2008 (20081016/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

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<http://www.cas.org/legal/infopolicy.html>

'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> s L85 or L87

L89 10 L85 OR L87

=> dup rem L89 L88

FILE 'CAPLUS' ENTERED AT 10:18:05 ON 17 OCT 2008  
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COPYRIGHT (C) 2008 THOMSON REUTERS  
PROCESSING COMPLETED FOR L89  
PROCESSING COMPLETED FOR L88  
L90 11 DUP REM L89 L88 (3 DUPLICATES REMOVED)

10/595943

ANSWERS '1-10' FROM FILE CAPLUS  
ANSWER '11' FROM FILE MEDLINE

=> d ibib abs L90 1-10; d iall L90 11

L90 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 1

ACCESSION NUMBER: 2007:667806 CAPLUS Full-text

DOCUMENT NUMBER: 147:257498

TITLE: A new chemoselective synthesis of brombuterol

AUTHOR(S): Nery, Marcelo S.; Azevedo, Mariangela S.; Cardoso, Jari N.; Slana, Glaucia B. C.; Lopes, Rosangela S. C.; Lopes, Claudio C.

CORPORATE SOURCE: Departamento de Quimica Analitica, Instituto de Quimica, Universidade Federal do Rio de Janeiro, Rio de Janeiro, CEP 21949 900, Brazil

SOURCE: Synthesis (2007), (10), 1471-1474

CODEN: SYNTBF; ISSN: 0039-7881

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 147:257498

AB A practical method for the synthesis of brombuterol [1-(4-amino-3,5-dibromophenyl)-2-(tert-butylamino)ethanol] in high overall yield is described starting from 4'-aminoacetophenone using a new chemoselective route.

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L90 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 2005:493567 CAPLUS Full-text

DOCUMENT NUMBER: 143:26622

TITLE: Hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids

INVENTOR(S): Lopes, Claudio Cerqueira; Lopes, Rosangela Sabattini Capella; Cardoso, Jari Nobrega; Alves Da Silva, Jacqueline; Ferreira Gomes, Leticia

PATENT ASSIGNEE(S): Universidade Federal do Rio de Janeiro-UFRJ, Brazil

SOURCE: PCT Int. Appl., 14 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005051870	A2	20050609	WO 2004-BR236	20041125
WO 2005051870	A3	20050707		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
BR 2003007864	A	20050705	BR 2003-7864	20031125
US 20070128680	A1	20070607	US 2006-595943	20060522

10/595943

PRIORITY APPLN. INFO.:

BR 2003-7864

A 20031125

WO 2004-BR236

W 20041125

OTHER SOURCE(S): CASREACT 143:26622; MARPAT 143:26622

AB A process to form hydrazides (e.g., luminol) from the reaction of a hydrazine and a dicarboxylic (e.g., 3-nitrophthalic acid) using a Lewis acid catalyst (e.g., niobium pentachloride) is described. The reaction occurs in a safe reactional environment, utilizing smooth conditions, neither involving high temps. nor high pressures, producing the desired products with high yields, between 90-95%. The invention also describes a kit for utilization of chemiluminescent substances, comprised of two solns.

L90 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 3

ACCESSION NUMBER: 2004:514933 CAPLUS Full-text

DOCUMENT NUMBER: 141:174024

TITLE: Synthesis of benzo[b]naphtho[2,3-d]furan-6,11-dione via one-pot remote anionic Fries rearrangement and metalation reaction

AUTHOR(S): Azevedo, Mariangela S.; Alves, Glaucia B. C.; Cardoso, Jari N.; Lopes, Rosangela S. C.; Lopes, Claudio C.

CORPORATE SOURCE: Instituto de Quimica, Departamento de Quimica Organica, CT, Universidade Federal do Rio de Janeiro, Rio de Janeiro, 21949 900, Brazil

SOURCE: Synthesis (2004), (8), 1262-1268

CODEN: SYNTBF; ISSN: 0039-7881

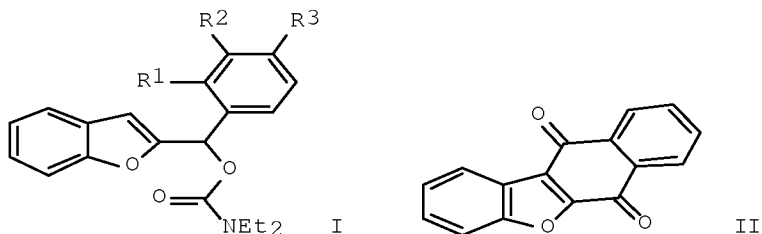
PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:174024

GI



AB The use of a lithiation reaction to transform the arylcarbamate I (R1 = Br; R2= R3 = H) into the corresponding benzo[b]naphtho[2,3-d]furan-6,11-dione II is described. I (R1 = H; R2 = R3 = OMe; R2R3 = OCH2O) underwent the anionic Fries rearrangement, when reacted with s-butyllithium, to give the corresponding carboxamidoaryl carbinols.

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L90 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

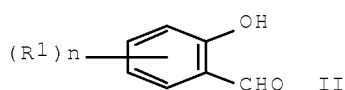
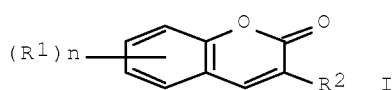
ACCESSION NUMBER: 2006:299566 CAPLUS Full-text

DOCUMENT NUMBER: 144:331264

10/595943

TITLE: Process for the preparation of substituted coumarin derivatives  
 INVENTOR(S): Carvalho, Jose Roque Mota; Lopes, Claudio Cerqueira; Lopes, Rosangela Sabattini Capella; Cardoso, Jari Nobrega; Slana, Glaucia Barbosa Alves; Guerra, Maicon  
 PATENT ASSIGNEE(S): Universidade Federal do Rio de Janeiro - UFRJ, Brazil  
 SOURCE: PCT Int. Appl., 14 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006032120	A2	20060330	WO 2005-BR188	20050920
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
BR 2004004130	A	20060502	BR 2004-4130	20040920
US 20080011985	A1	20080117	US 2007-574845	20070307
PRIORITY APPLN. INFO.:			BR 2004-4130	A 20040920
			WO 2005-BR188	W 20050920
OTHER SOURCE(S):		MARPAT 144:331264		
GI				

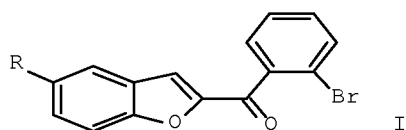


AB A process for the preparation of coumarin derivs., such as I [R1 = OH, CN, alkyl, alkenyl, alkynyl, aryl, acyl, halogen, dialkylamino, etc.; R2 = alkyl, alkenyl, alkynyl, etc.; n = 1, 2, 3, or 4], via cyclocondensation of corresponding 2-hydroxybenzaldehyde derivs. II with carboxylic acids R2CO2H. These coumarin derivs. are fluorescent when irradiated by UV light.

L90 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2006:1289630 CAPLUS Full-text  
 DOCUMENT NUMBER: 147:406621  
 TITLE: A novel synthesis of  $\alpha$ -bromoacetophenones and its application in obtaining 2-benzoylbenzofurans  
 AUTHOR(S): Azevedo, Mariangela S.; Alves, Ana Paula L.; Alves,

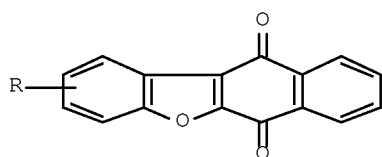
10/595943

Glaucia B. C.; Cardoso, Jari N.; Lopes, Rosangela S. C.; Lopes, Claudio C.  
CORPORATE SOURCE: Departamento de Quimica Analitica, Instituto de Quimica, Universidade Federal do Rio de Janeiro, Rio de Janeiro, 21949-900, Brazil  
SOURCE: Quimica Nova (2006), 29(6), 1259-1265  
CODEN: QUNODK; ISSN: 0100-4042  
PUBLISHER: Sociedade Brasileira de Quimica  
DOCUMENT TYPE: Journal  
LANGUAGE: Portuguese  
OTHER SOURCE(S): CASREACT 147:406621  
GI

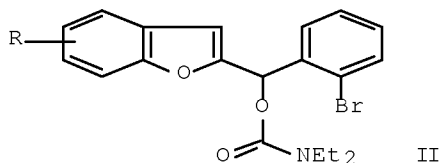


AB  $\alpha$ -Bromoacetophenones are important in organic synthesis. They have been widely used as precursors of several natural products. Several methods of their synthesis via bromination have been described, however they furnish a mixture of starting material, mono and dibromide products. A novel, simple and efficient synthesis of these compds. have been developed and further applied to the preparation of benzoylbenzofurans, e.g., I (R = H or MeO). Benzoylbenzofurans are compds. with important pharmacol. properties, such as the ability of dilating the coronary artery and analgesic action. Such compds. have also been used as key intermediates to obtain quinone systems.  
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L90 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2006:301972 CAPLUS Full-text  
DOCUMENT NUMBER: 146:316668  
TITLE: Total syntheses of oxygenated brazanquinones via regioselective homologous anionic Fries rearrangement of benzylic O-carbamates  
AUTHOR(S): Slana, Glaucia G. B. C. A. S.; Azevedo, Mariangela M. S. A.; Cardoso, Jari J. N. C.; Lopes, Rosangela R. S. C. L.; Lopes, Claudio C. C. L.  
CORPORATE SOURCE: Instituto de Quimica, Universidade Federal do Rio de Janeiro, Rio de Janeiro, 21949-900, Brazil  
SOURCE: Beilstein Journal of Organic Chemistry (2006), 2(Feb.), No pp. given  
CODEN: BJOCBH; ISSN: 1860-5397  
URL: <http://bjoc.beilstein-journals.org/content/pdf/1860-5397-2-1.pdf>  
PUBLISHER: Beilstein-Institut zur Foerderung der Chemischen Wissenschaften  
DOCUMENT TYPE: Journal; (online computer file)  
LANGUAGE: English  
GI



I



II

AB Using new variations of anionic aromatic chemical, the total synthesis of oxygenated brazanquinones I [R = 8-OMe, 7-OMe, 6-OMe], derived from  $\beta$ -brasan, a natural product isolated from *Caesalpinia echinata*, via carbamates II is described.

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L90 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:1357896 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 146:45735

TITLE: Process for the preparation of aspartame derivative

INVENTOR(S): Costa da Silva, Jaciara; Lopes, Claudio Cerqueira; Lopes, Rosangela Sabattini Capella; Cardoso, Jari Nobrega; Albert, Andre Luis Mazzei

PATENT ASSIGNEE(S): Universidade Federal do Rio de Janeiro - Ufrj, Brazil

SOURCE: Braz. Pedido PI, 14pp.

CODEN: BPXXDX

DOCUMENT TYPE: Patent

LANGUAGE: Portuguese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BR 2004000467	A	20051116	BR 2004-467	20040308
PRIORITY APPLN. INFO.:			BR 2004-467	20040308

OTHER SOURCE(S): CASREACT 146:45735; MARPAT 146:45735

AB The invention relates to aspartame derivs. RO2C-L-Asp-L-Phe-OMe (R is C1-8 alkyl) or acceptable salts, which are sweet and have improved thermal stability. Thus, treatment of aspartame with (tert-butoxycarbonyloxyimino)phenylacetonitrile (Boc-ON) in aqueous dioxane in the presence of triethylamine afforded Boc-aspartame.

L90 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:52767 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 139:358454

TITLE: Pyrazolinone-piperidine dipeptide growth hormone

secretagogues (GHSs): discovery of capromorelin  
 AUTHOR(S): Carpino, Philip A.; Lefker, Bruce A.; Toler, Steven M.; Pan, Lydia C.; Hadcock, John R.; Cook, Ewell R.; DiBrino, Joseph N.; Campeta, Anthony M.; DeNinno, Shari L.; Chidsey-Frink, Kristin L.; Hada, William A.; Inthavongsay, John; Mangano, F. Michael; Mullins, Michelle A.; Nickerson, David F.; Ng, Oicheng; Pirie, Christine M.; Ragan, John A.; Rose, Colin R.; Tess, David A.; Wright, Ann S.; Yu, Li; Zawistoski, Michael P.; DaSilva-Jardine, Paul A.; Wilson, Theresa C.;

10/595943

Thompson, David D.  
CORPORATE SOURCE: Groton Labs, Pfizer Global Research and Development,  
Groton, CT, 06340, USA  
SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(4),  
581-590  
CODEN: BMECEP; ISSN: 0968-0896  
PUBLISHER: Elsevier Science Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 139:358454  
AB Novel pyrazolinone-piperidine dipeptide derivs. were synthesized and evaluated  
as growth hormone secretagogues (GHSs). Two analogs, capromorelin (5, CP-  
424391-18, hGHS-R1a Ki=7 nM, rat pituicyte EC50=3 nM) and the des-Me analog 5c  
(hGHS-R1a Ki=17 nM, rat pituicyte EC50=3 nM), increased plasma GH levels in an  
anesthetized rat model, with ED50 values less than 0.05 mg/kg iv.  
Capromorelin showed enhanced intestinal absorption in rodent models and  
exhibited superior pharmacokinetic properties, including high  
bioavailabilities in two animal species [F(rat)=65%, F(dog)=44%]. This short-  
duration GHS was orally active in canine models and was selected as a  
development candidate for the treatment of musculoskeletal frailty in elderly  
adults.  
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L90 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:808833 CAPLUS Full-text

DOCUMENT NUMBER: 138:378539

TITLE: Discovery and biological characterization of  
capromorelin analogues with extended half-lives

AUTHOR(S): Carpino, Philip A.; Lefker, Bruce A.; Toler, Steven  
M.; Pan, Lydia C.; Hadcock, John R.; Murray, Marianne  
C.; Cook, Ewell R.; Di Brino, Joseph N.; De Ninno,  
Shari L.; Chidsey-Frink, Kristin L.; Hada, William A.;  
Inthavongsay, John; Lewis, Sharon K.; Mangano, F.  
Michael; Mullins, Michelle A.; Nickerson, David F.;  
Ng, Oicheng; Pirie, Christine M.; Ragan, John A.;  
Rose, Colin R.; Tess, David A.; Wright, Ann S.; Yu,  
Li; Zawistoski, Michael P.; Pettersen, John C.; Da  
Silva-Jardine, Paul A.; Wilson, Theresa C.; Thompson,  
David D.

CORPORATE SOURCE: Groton Labs, Pfizer Global Research & Development,  
Groton, CT, 06340, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2002),  
12(22), 3279-3282

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:378539

AB New tert-Bu, picolyl and fluorinated analogs of capromorelin, a short-acting  
growth hormone secretagogue (GHS), were prepared as part of a program to  
identify long-acting GHSs that increase 24-h plasma IGF-1 levels. Some  
compsds. (ACD LogD values  $\geq 2.9$ ) displayed extended plasma elimination half-  
lives in dogs, primarily due to high vols. of distribution, but showed weak GH  
secretagogue activities in rats (ED50s > 10 mg/kg). A less lipophilic  
derivative CP-464709-18 (ACD LogD=1.6) exhibited a shorter canine half-life,  
but stimulated GH secretion in two animal species. Repeat oral dosing of CP-  
464709-18 to dogs for 29 days (6 mg/kg) resulted in a significant down-  
regulation of the post dose GH response and a 60 and 40% increase in IGF-1

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levels relative to pre-dose levels at the 8- and 24-h post dose time points.  
CP-464709-18 was selected as a candidate for the treatment of frailty.

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L90 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:858884 CAPLUS Full-text

DOCUMENT NUMBER: 138:169800

TITLE: Study of the protonation/deprotonation sequence of two  
polyamines: bis-[(2S)-2-  
pyrrolidinylmethyl]ethylenediamine and spermidine by  
1H and 13C nuclear magnetic resonance

AUTHOR(S): Da Silva, Jacqueline Alves; Felcman, Judith; Lopes,  
Claudio Cerqueira; Lopes, Rosangela S. C.; Villar,  
Jose Daniel Figueroa

CORPORATE SOURCE: Department of Chemistry, Pontificia Universidade  
Catolica do Rio de Janeiro, PUC, Rio de Janeiro,  
Brazil

SOURCE: Spectroscopy Letters (2002), 35(5), 643-661

CODEN: SPLEBX; ISSN: 0038-7010

PUBLISHER: Marcel Dekker, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:169800

AB In this paper we describe the study of protonation/deprotonation of two  
polyamines: bis[(2S)-2-pyrrolidinylmethyl]ethylenediamine (tetra) and  
spermidine (Spd). A new synthetic route was established for the synthesis of  
tetra, which structure was confirmed by IR, elemental anal., 1H-NMR, 13C-  
NMR(Pendant) and 2D-NMR (COSY, 13C-1H HETCOR and HMQC) spectra. The  
protonation/deprotonation sequence studies of tetra and Spd were determined by  
potentiometric and NMR methods. For the NMR studies, the tetra and Spd  
samples were dissolved in D2O and the pD adusted with NaOD. The  
protonation/deprotonation sequences of tetra and Spd were determined by means  
of the values and the variations of the hydrogen atom and 13C NMR chemical  
shifts as a function of hydrogen atom pD. The variation of  $\delta 1H$  with pD  
clearly showed that the first protonation of tetra occurs at the pyrrolidine  
nitrogen atoms and the second protonation occurs at the ethylenediamine  
nitrogen atom. The anal. of the 13C-NMR spectra confirmed the results  
obtained by 1H-NMR, as a greater chemical shift variation was observed for C-6  
(5.6 ppm), as compared to C-8 (1.8 ppm). In the study with Spd, the greater  
chemical shift variation was observed for C-2 (6.75 ppm) and C-5 (4.95 ppm),  
indicating that the deprotonation occurs first at the secondary nitrogen atoms  
and the second and third deprotonation steps occur at the primary nitrogen  
atoms.

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L90 ANSWER 11 OF 11 MEDLINE on STN

ACCESSION NUMBER: 2006162323 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 16542010

TITLE: Total syntheses of oxygenated brazanquinones via  
regioselective homologous anionic Fries rearrangement of  
benzylic O-carbamates.

AUTHOR: Slana Glaucia Barbosa Candido Alves; de Azevedo Mariangela  
Soares; Lopes Rosangela Sabattini Capella; Lopes Claudio  
Cerqueira; Cardoso Jari Nobrega

CORPORATE SOURCE: Instituto de Quimica, Universidade Federal do Rio de



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Janeiro, CT, Bl A/508, 21949-900 Rio de Janeiro - RJ,  
Brazil.. glaucia@gmx.net  
SOURCE: Beilstein journal of organic chemistry, (2006) Vol. 2, No.  
1, pp. 1. Electronic Publication: 2006-02-21.  
Journal code: 101250746. E-ISSN: 1860-5397.  
PUB. COUNTRY: Germany: Germany, Federal Republic of  
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)  
LANGUAGE: English  
FILE SEGMENT: NONMEDLINE; PUBMED-NOT-MEDLINE  
ENTRY MONTH: 200604  
ENTRY DATE: Entered STN: 23 Mar 2006  
Last Updated on STN: 27 Apr 2006  
Entered Medline: 26 Apr 2006

ABSTRACT:

Using new variations of anionic aromatic chemistry, the total synthesis of oxygenated brazanquinones (1a-1c), derived from beta-brasan, a natural product isolated from *Caesalpinia echinata*, via carbamates 2a-2c is described.

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DICTIONARY FILE UPDATES: 15 OCT 2008 HIGHEST RN 1061881-29-5

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FILE CONTENT:1840 - 12 Oct 2008 VOL 149 ISS 16

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=> d stat que L43

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L6 STR

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Structure attributes must be viewed using STN Express query preparation.

L8 446 SEA FILE=CASREACT SSS FUL L6 ( 4732 REACTIONS)

L42 152 SEA FILE=CASREACT ABB=ON PLU=ON 10026-12-7

L43 1 SEA FILE=CASREACT ABB=ON PLU=ON L42 (L) L8

=> d ibib abs hit L43 1

L43 ANSWER 1 OF 1 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 143:26622 CASREACT Full-text

TITLE: Hydrazide catalytic production process from hydrazines  
and dicarboxylic acids in the presence of Lewis acids  
INVENTOR(S): Lopes, Claudio Cerqueira; Lopes, Rosangela Sabattini  
Capella; Cardoso, Jari Nobrega; Alves Da Silva,  
Jacqueline; Ferreira Gomes, Leticia

PATENT ASSIGNEE(S): Universidade Federal do Rio de Janeiro-UFRJ, Brazil

SOURCE: PCT Int. Appl., 14 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

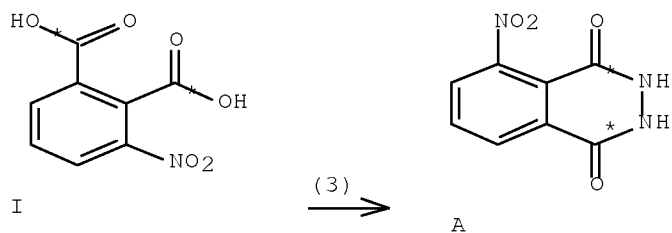
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005051870	A2	20050609	WO 2004-BR236	20041125
WO 2005051870	A3	20050707		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
BR 2003007864	A	20050705	BR 2003-7864	20031125
US 20070128680	A1	20070607	US 2006-595943	20060522
PRIORITY APPLN. INFO.:			BR 2003-7864	20031125
			WO 2004-BR236	20041125

OTHER SOURCE(S): MARPAT 143:26622

AB A process to form hydrazides (e.g., luminol) from the reaction of a hydrazine and a dicarboxylic (e.g., 3-nitrophthalic acid) using a Lewis acid catalyst (e.g., niobium pentachloride) is described. The reaction occurs in a safe reactional environment, utilizing smooth conditions, neither involving high temps. nor high pressures, producing the desired products with high yields, between 90-95%. The invention also describes a kit for utilization of chemiluminescent substances, comprised of two solns.

RX(3) OF 6 ...I ==> A...

10/595943



RX(3) RCT I 603-11-2

STAGE(1)

CAT 10026-12-7 NbCl5

CON 30 minutes, room temperature

STAGE(2)

RGT L 302-01-2 N2H4

SOL 7732-18-5 Water

CON SUBSTAGE(1) 30 minutes, room temperature -> 50 deg C

SUBSTAGE(2) 4 hours, 50 deg C

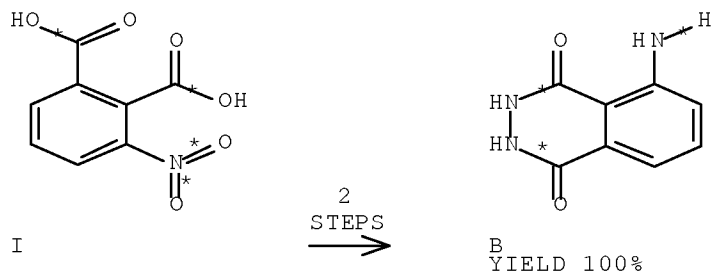
SUBSTAGE(3) cooled

PRO A 3682-15-3

NTE inert

RX(5) OF 6 COMPOSED OF RX(3), RX(1)

RX(5) I ==> E



RX(3) RCT I 603-11-2

STAGE(1)

CAT 10026-12-7 NbCl5

CON 30 minutes, room temperature

STAGE(2)

RGT L 302-01-2 N2H4

SOL 7732-18-5 Water

CON SUBSTAGE(1) 30 minutes, room temperature -> 50 deg C

10/595943

SUBSTAGE(2) 4 hours, 50 deg C  
SUBSTAGE(3) cooled

PRO A 3682-15-3  
NTE inert

RX(1) RCT A 3682-15-3  
RGT C 1333-74-0 H2  
PRO B 521-31-3  
CAT 7440-05-3 Pd  
SOL 123-91-1 Dioxane, 7732-18-5 Water, 64-19-7 AcOH  
CON room temperature  
NTE Pd supported on carbon was used as catalyst, sodium dithionite  
in acidic medium can also be used as reducing agent

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=> file registry

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FILE CONTENT:1840 - 12 Oct 2008 VOL 149 ISS 16

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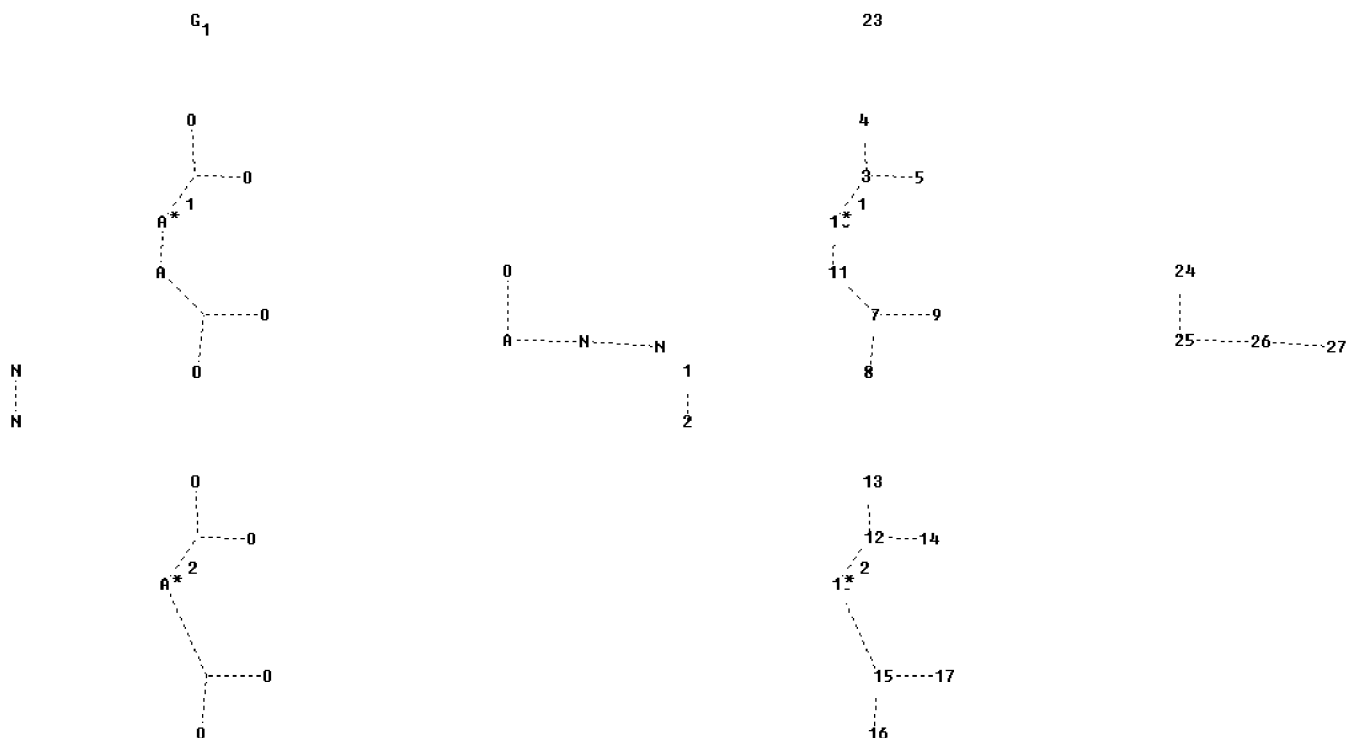
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```
chain nodes :
3 4 5 7 8 9 12 13 14 15 16 17 23 24
ring/chain nodes :
1 2 10 11 18 25 26 27
chain bonds :
3-4 3-5 3-10 7-8 7-9 7-11 12-13 12-14 12-18 15-16 15-17 15-18 24-25

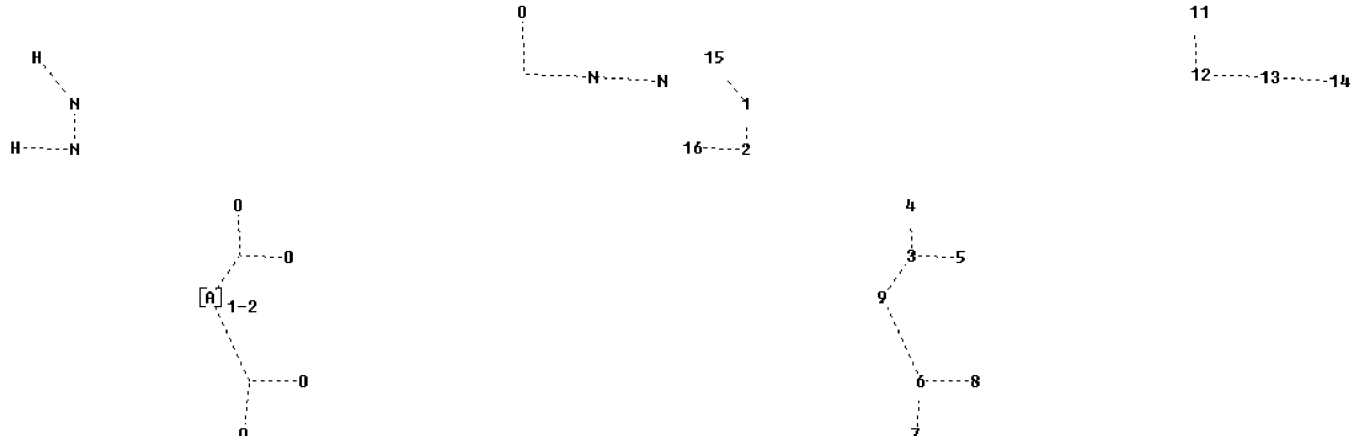
ring/chain bonds :
1-2 10-11 25-26 26-27
exact/norm bonds :
1-2 3-4 3-5 3-10 7-8 7-9 7-11 10-11 12-13 12-14 12-18 15-16 15-17 15-18
24-25 25-26 26-27
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G1:[\*1],[\*2]

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Connectivity :
3:3 E exact RC ring/chain 4:1 E exact RC ring/chain 5:1 E exact RC ring/chain
7:3 E exact RC ring/chain 8:1 E exact RC ring/chain 9:1 E exact RC ring/chain
12:3 E exact RC ring/chain
13:1 E exact RC ring/chain 14:1 E exact RC ring/chain 15:3 E exact RC ring/chain
16:1
E exact RC ring/chain 17:1 E exact RC ring/chain 24:1 E exact RC ring/chain
Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
23:CLASS 24:CLASS
25:CLASS 26:CLASS 27:CLASS
fragments assigned product role:
containing 24
fragments assigned reactant/reagent role:
containing 1
containing 23
```

10/595943

Uploading L59.str



```
chain nodes :
4 5 7 8 11 15 16
ring/chain nodes :
1 2 3 6 9 12 13 14
chain bonds :
1-15 2-16 3-4 3-5 6-7 6-8 11-12
ring/chain bonds :
1-2 3-9 6-9 12-13 13-14
exact/norm bonds :
1-2 1-15 2-16 3-4 3-5 3-9 6-7 6-8 6-9 11-12 12-13 13-14
```

```
Connectivity :
3:3 E exact RC ring/chain 4:1 E exact RC ring/chain 5:1 E exact RC ring/chain
6:3 E exact RC ring/chain 7:1 E exact RC ring/chain 8:1 E exact RC ring/chain
11:1 E exact RC ring/chain
```

```
Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS
fragments assigned reactant role:
containing 3
fragments assigned product role:
containing 11
fragments assigned reactant/reagent role:
containing 1
reaction site bonds:
12-13:CC
node mappings:
3:12 1:13
```

```
=> d stat que L62
L6 STR
```

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Structure attributes must be viewed using STN Express query preparation.

L8 446 SEA FILE=CASREACT SSS FUL L6 ( 4732 REACTIONS)  
L20 2766 SEA FILE=CASREACT ABB=ON PLU=ON LEWIS ACID?/CW  
L59 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

L61 163 SEA FILE=CASREACT SUB=L8 SSS FUL L59 ( 1426 REACTIONS)  
L62 1 SEA FILE=CASREACT ABB=ON PLU=ON L61 AND L20

=> d stat que L63

L6 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

L8 446 SEA FILE=CASREACT SSS FUL L6 ( 4732 REACTIONS)  
L21 9688 SEA FILE=CASREACT ABB=ON PLU=ON LEWIS ACID?/BI,NTE  
L59 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

L61 163 SEA FILE=CASREACT SUB=L8 SSS FUL L59 ( 1426 REACTIONS)  
L63 1 SEA FILE=CASREACT ABB=ON PLU=ON L61 AND L21

=> d stat que L64

L2 28 SEA FILE=REGISTRY ABB=ON PLU=ON (10025-73-7/BI OR 10025-91-9/  
BI OR 10026-07-0/BI OR 10026-10-5/BI OR 10026-11-6/BI OR  
10026-12-7/BI OR 10049-06-6/BI OR 10108-64-2/BI OR 10294-34-5/B  
I OR 13450-90-3/BI OR 22441-45-8/BI OR 7446-70-0/BI OR  
7447-39-4/BI OR 7487-94-7/BI OR 7550-45-0/BI OR 7637-07-2/BI  
OR 7646-79-9/BI OR 7646-85-7/BI OR 7647-18-9/BI OR 7705-07-9/BI  
OR 7705-08-0/BI OR 7718-54-9/BI OR 7758-89-6/BI OR 7784-34-1/B  
I OR 7786-30-3/BI OR 7787-47-5/BI OR 7787-60-2/BI OR 7789-48-2/  
BI)  
L6 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

L8 446 SEA FILE=CASREACT SSS FUL L6 ( 4732 REACTIONS)  
L12 TRANSFER PLU=ON L8 1- RX : 5601 TERMS  
L13 5601 SEA FILE=REGISTRY ABB=ON PLU=ON L12/RN  
L14 11 SEA FILE=REGISTRY ABB=ON PLU=ON L13 AND L2  
L15 348 SEA FILE=REGISTRY ABB=ON PLU=ON L13 AND (M/ELS OR B/ELS OR  
AS/ELS OR TE/ELS OR AT/ELS)  
L16 97 SEA FILE=REGISTRY ABB=ON PLU=ON L15 AND X/ELS  
L17 86 SEA FILE=REGISTRY ABB=ON PLU=ON L16 NOT L14  
L18 62 SEA FILE=REGISTRY ABB=ON PLU=ON L17 AND C/ELS  
L19 24 SEA FILE=REGISTRY ABB=ON PLU=ON L17 NOT L18  
L29 35 SEA FILE=REGISTRY ABB=ON PLU=ON L14 OR L19  
L30 106670 SEA FILE=CASREACT ABB=ON PLU=ON L29  
L59 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

10/595943

Structure attributes must be viewed using STN Express query preparation.

L61 163 SEA FILE=CASREACT SUB=L8 SSS FUL L59 ( 1426 REACTIONS)  
L64 30 SEA FILE=CASREACT ABB=ON PLU=ON L61 (L) L30

=> d stat que L65

L2 28 SEA FILE=REGISTRY ABB=ON PLU=ON (10025-73-7/BI OR 10025-91-9/  
BI OR 10026-07-0/BI OR 10026-10-5/BI OR 10026-11-6/BI OR  
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I OR 13450-90-3/BI OR 22441-45-8/BI OR 7446-70-0/BI OR  
7447-39-4/BI OR 7487-94-7/BI OR 7550-45-0/BI OR 7637-07-2/BI  
OR 7646-79-9/BI OR 7646-85-7/BI OR 7647-18-9/BI OR 7705-07-9/BI  
OR 7705-08-0/BI OR 7718-54-9/BI OR 7758-89-6/BI OR 7784-34-1/B  
I OR 7786-30-3/BI OR 7787-47-5/BI OR 7787-60-2/BI OR 7789-48-2/  
BI)  
L6 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

L8 446 SEA FILE=CASREACT SSS FUL L6 ( 4732 REACTIONS)  
L12 TRANSFER PLU=ON L8 1- RX : 5601 TERMS  
L13 5601 SEA FILE=REGISTRY ABB=ON PLU=ON L12/RN  
L14 11 SEA FILE=REGISTRY ABB=ON PLU=ON L13 AND L2  
L15 348 SEA FILE=REGISTRY ABB=ON PLU=ON L13 AND (M/ELS OR B/ELS OR  
AS/ELS OR TE/ELS OR AT/ELS)  
L16 97 SEA FILE=REGISTRY ABB=ON PLU=ON L15 AND X/ELS  
L17 86 SEA FILE=REGISTRY ABB=ON PLU=ON L16 NOT L14  
L18 62 SEA FILE=REGISTRY ABB=ON PLU=ON L17 AND C/ELS  
L31 15382 SEA FILE=CASREACT ABB=ON PLU=ON L18/CAT  
L59 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

L61 163 SEA FILE=CASREACT SUB=L8 SSS FUL L59 ( 1426 REACTIONS)  
L65 2 SEA FILE=CASREACT ABB=ON PLU=ON L61 (L) L31

=> s L62 or L63 or L64 or L65

L91 30 L62 OR L63 OR L64 OR L65

=> d ibib abs hit L91 1-30

L91 ANSWER 1 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 148:168645 CASREACT Full-text

TITLE: Iptycene-Derived Pyridazines and Phthalazines

AUTHOR(S): Bouffard, Jean; Eaton, Robert F.; Mueller, Peter;  
Swagger, Timothy M.

CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of  
Technology, Cambridge, MA, 02139, USA

SOURCE: Journal of Organic Chemistry (2007), 72(26),  
10166-10180

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

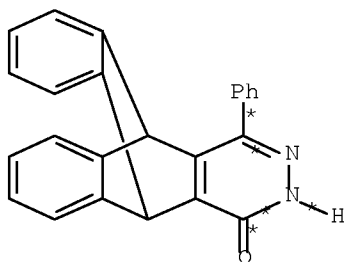
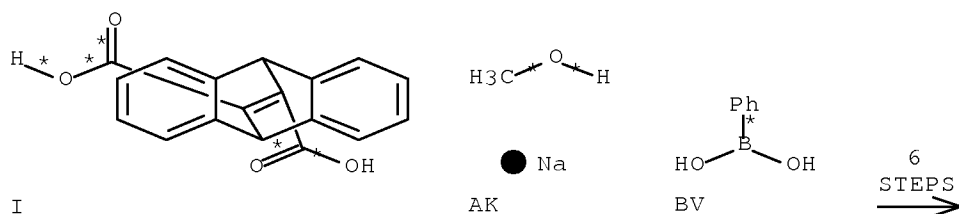
AB The synthesis of new heterocyclic oligo(phenylene) analogs based on soluble,  
non-aggregating 1,2-diazines is reported. Improved palladium-catalyzed

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reductive coupling methods were developed to allow for the preparation of large quantities of iptycene-derived bipyridazine compds. and biphthalazine compds., and the controlled synthesis of well-defined oligomers up to sexipyridazine. Crystallog., spectroscopic, and computational evidence indicate that in these analogs, hindrance at the ortho position is relaxed relative to poly(phenylenes). The resulting building blocks are promising for incorporation in conjugated electronics materials and as new iptycene-derived ligands for transition metals.

REFERENCE COUNT: 113 THERE ARE 113 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

RX(279) OF 371 COMPOSED OF RX(7), RX(10), RX(13), RX(18), RX(41), RX(45)  
RX(279) I + AK + BV ==> CR



CR  
YIELD 72%

RX(7) RCT I 1625-81-6

STAGE(1)

CAT 68-12-2 DMF  
SOL 75-09-2 CH2Cl2  
CON room temperature -> 0 deg C

STAGE(2)

RGT Q 79-37-8 (COCl)2  
CON overnight, 0 deg C -> room temperature

PRO P 1625-83-8

RX(10) RCT P 1625-83-8

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RGT W 2644-70-4 Hydrazine, hydrochloride (1:1)  
 PRO V 937081-42-0  
 SOL 64-19-7 AcOH  
 CON SUBSTAGE(1) overnight, reflux  
 SUBSTAGE(2) reflux -> room temperature

RX(13) RCT V 937081-42-0

STAGE(1)

RGT AB 10025-87-3 POC13  
 CON SUBSTAGE(1) overnight, reflux  
 SUBSTAGE(2) reflux -> room temperature

STAGE(2)

RGT AC 1344-28-1 Al2O3  
 SOL 75-09-2 CH2Cl2  
 CON 1 hour, room temperature

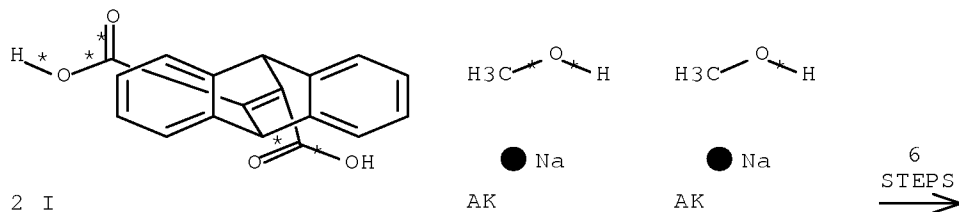
PRO AA 937081-43-1

RX(18) RCT AA 937081-43-1, AK 124-41-4  
 PRO AL 937081-49-7  
 SOL 109-99-9 THF  
 CON 22 hours, room temperature  
 NTE chemoselective

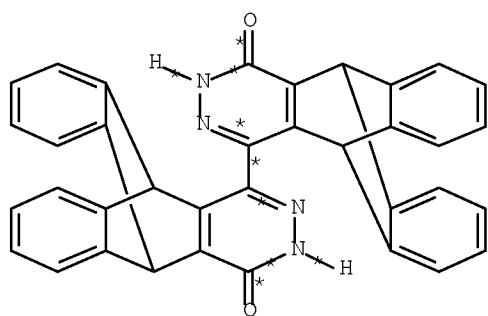
RX(41) RCT AL 937081-49-7, BV 98-80-6  
 RGT BS 13400-13-0 CsF  
 PRO CK 937081-50-0  
 CAT 14221-01-3 Pd(PPh3)4  
 SOL 123-91-1 Dioxane  
 CON SUBSTAGE(1) 48 hours, 115 deg C  
 SUBSTAGE(2) 115 deg C -> room temperature  
 NTE Suzuki coupling

RX(45) RCT CK 937081-50-0  
 RGT CS 10035-10-6 HBr  
 PRO CR 1001639-89-9  
 SOL 64-19-7 AcOH  
 CON SUBSTAGE(1) overnight, 90 deg C  
 SUBSTAGE(2) 90 deg C -> room temperature  
 NTE violent release of gases (HBr, MeBr) occurs on warming the reaction, safety

RX(281) OF 371 COMPOSED OF RX(7), RX(10), RX(13), RX(18), RX(50), RX(53)  
 RX(281) 2 I + 2 AK ==> DH



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DH  
YIELD 91%

RX(7) RCT I 1625-81-6

STAGE(1)  
CAT 68-12-2 DMF  
SOL 75-09-2 CH2Cl2  
CON room temperature -> 0 deg C

STAGE(2)  
RGT Q 79-37-8 (COCl)2  
CON overnight, 0 deg C -> room temperature

PRO P 1625-83-8

RX(10) RCT P 1625-83-8  
RGT W 2644-70-4 Hydrazine, hydrochloride (1:1)  
PRO V 937081-42-0  
SOL 64-19-7 AcOH  
CON SUBSTAGE(1) overnight, reflux  
SUBSTAGE(2) reflux -> room temperature

RX(13) RCT V 937081-42-0

STAGE(1)  
RGT AB 10025-87-3 POCl3  
CON SUBSTAGE(1) overnight, reflux  
SUBSTAGE(2) reflux -> room temperature

STAGE(2)  
RGT AC 1344-28-1 Al2O3  
SOL 75-09-2 CH2Cl2  
CON 1 hour, room temperature

PRO AA 937081-43-1

RX(18) RCT AA 937081-43-1, AK 124-41-4  
PRO AL 937081-49-7  
SOL 109-99-9 THF  
CON 22 hours, room temperature  
NTE chemoselective

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RX(50) RCT AL 937081-49-7

STAGE(1)

RGT DA 7440-66-6 Zn  
CAT 603-35-0 PPh3, 13965-03-2 PdCl2(PPh3)2  
SOL 68-12-2 DMF  
CON 20 hours, 100 deg C

STAGE(2)

RGT DB 139-33-3 Di-Na EDTA  
SOL 7732-18-5 Water

PRO CZ 1001639-98-0

RX(53) RCT CZ 1001639-98-0

STAGE(1)

RGT CS 10035-10-6 HBr  
SOL 64-19-7 AcOH  
CON SUBSTAGE(1) overnight, 90 deg C  
SUBSTAGE(2) 90 deg C -> room temperature

STAGE(2)

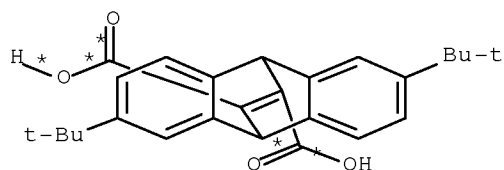
RGT CY 127-09-3 AcONa  
SOL 7732-18-5 Water

PRO DH 1001640-06-7

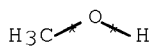
NTE violent release of gases (HBr, MeBr) occurs on warming the reaction, safety

RX(289) OF 371 COMPOSED OF RX(8), RX(11), RX(14), RX(19), RX(51), RX(54)

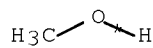
RX(289) 4 N + 4 AK ==> DI + DJ



4 N

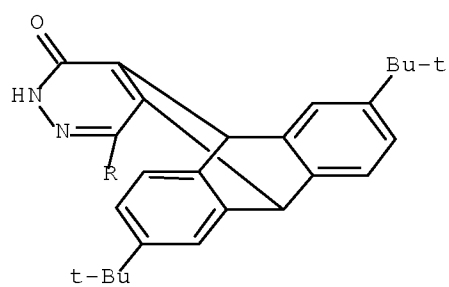
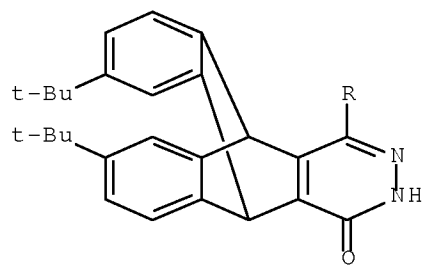


● Na  
AK

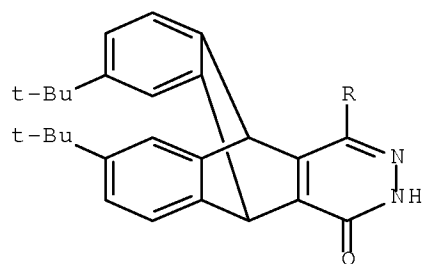


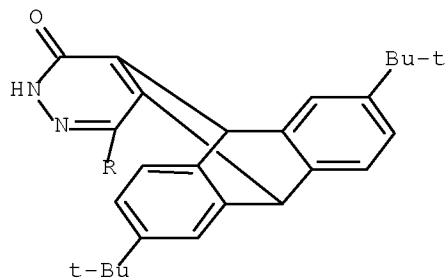
● Na  
3 AK

6  
STEPS  
→



DI  
YIELD 97% (50)





DJ  
YIELD 97% (50)

RX(8) RCT N 1001639-36-6

STAGE(1)

CAT 68-12-2 DMF  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON room temperature -> 0 deg C

STAGE(2)

RGT Q 79-37-8 (COCl)<sub>2</sub>  
CON overnight, 0 deg C -> room temperature

PRO T 1001639-38-8

RX(11) RCT T 1001639-38-8  
RGT W 2644-70-4 Hydrazine, hydrochloride (1:1)  
PRO Y 1001639-41-3  
SOL 64-19-7 AcOH  
CON SUBSTAGE(1) overnight, reflux  
SUBSTAGE(2) reflux -> room temperature

RX(14) RCT Y 1001639-41-3

STAGE(1)

RGT AB 10025-87-3 POCl<sub>3</sub>  
CON SUBSTAGE(1) overnight, reflux  
SUBSTAGE(2) reflux -> room temperature

STAGE(2)

RGT AC 1344-28-1 Al<sub>2</sub>O<sub>3</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 1 hour, room temperature

PRO AD 1001639-46-8

RX(19) RCT AD 1001639-46-8, AK 124-41-4  
PRO AN 1001639-50-4  
SOL 109-99-9 THF  
CON 48 hours, room temperature  
NTE chemoselective, reaction must be monitored by TLC to minimize formation of dimethoxy-substituted product or the isolation of unreacted starting material



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RX(51) RCT AN 1001639-50-4

STAGE(1)

RGT DA 7440-66-6 Zn  
CAT 603-35-0 PPh3, 13965-03-2 PdCl2(PPh3)2  
SOL 68-12-2 DMF  
CON 20 hours, 100 deg C

STAGE(2)

RGT DB 139-33-3 Di-Na EDTA  
SOL 7732-18-5 Water  
CON 1 hour, room temperature

PRO DE 1001898-97-0, DF 1001899-70-2

RX(54) RCT DE 1001898-97-0, DF 1001899-70-2

STAGE(1)

RGT CS 10035-10-6 HBr  
SOL 64-19-7 AcOH  
CON SUBSTAGE(1) overnight, 95 deg C  
SUBSTAGE(2) 95 deg C -> room temperature

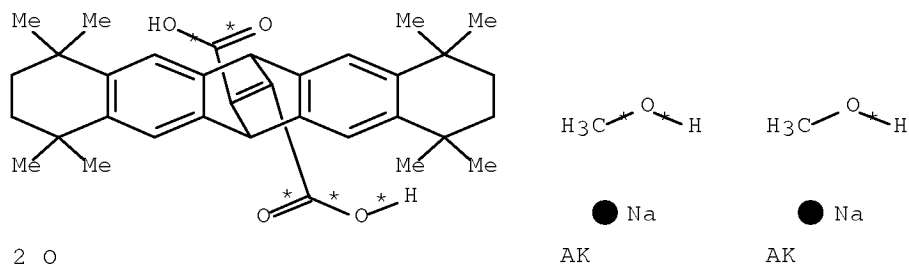
STAGE(2)

RGT CY 127-09-3 AcONa  
SOL 7732-18-5 Water

PRO DI 1001898-98-1, DJ 1001899-01-9

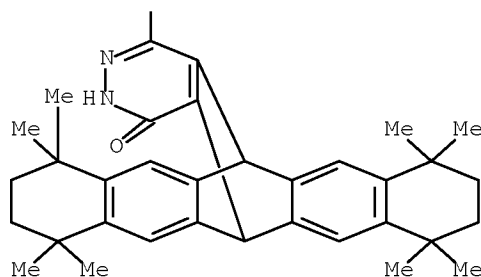
NTE violent release of gases (HBr, MeBr) occurs on warming the reaction, safety

RX(293) OF 371 COMPOSED OF RX(9), RX(12), RX(15), RX(20), RX(52), RX(55)  
RX(293) 2 O + 2 AK ==> DK



6  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*



DK  
YIELD 100%

RX(9) RCT O 1001639-37-7

STAGE(1)

CAT 68-12-2 DMF  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON room temperature -> 0 deg C

STAGE(2)

RGT Q 79-37-8 (COCl)<sub>2</sub>  
CON overnight, 0 deg C -> room temperature

PRO U 1001639-39-9

RX(12) RCT U 1001639-39-9  
RGT W 2644-70-4 Hydrazine, hydrochloride (1:1)  
PRO Z 1001639-43-5  
SOL 64-19-7 AcOH  
CON SUBSTAGE(1) overnight, reflux  
SUBSTAGE(2) reflux -> room temperature

RX(15) RCT Z 1001639-43-5

STAGE(1)

RGT AB 10025-87-3 POCl<sub>3</sub>  
CON SUBSTAGE(1) overnight, reflux  
SUBSTAGE(2) reflux -> room temperature

STAGE(2)

RGT AC 1344-28-1 Al<sub>2</sub>O<sub>3</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 1 hour, room temperature

PRO AE 1001639-47-9

RX(20) RCT AE 1001639-47-9, AK 124-41-4  
PRO AO 1001639-52-6  
SOL 109-99-9 THF  
CON overnight, room temperature  
NTE chemoselective, reaction must be monitored by TLC to minimize formation of dimethoxy-substituted product or the isolation of unreacted starting material

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RX(52) RCT AO 1001639-52-6

STAGE(1)

RGT DA 7440-66-6 Zn  
CAT 603-35-0 PPh3, 13965-03-2 PdCl2(PPh3)2  
SOL 68-12-2 DMF  
CON 40 hours, 100 deg C

STAGE(2)

RGT DB 139-33-3 Di-Na EDTA  
SOL 7732-18-5 Water  
CON 1 hour

PRO DG 1001640-05-6

RX(55) RCT DG 1001640-05-6

STAGE(1)

RGT CS 10035-10-6 HBr  
SOL 64-19-7 AcOH  
CON SUBSTAGE(1) overnight, 95 deg C  
SUBSTAGE(2) 95 deg C -> room temperature

STAGE(2)

RGT CY 127-09-3 AcONa  
SOL 7732-18-5 Water

PRO DK 1001640-10-3

NTE violent release of gases (HBr, MeBr) occurs on warming the reaction, safety

L91 ANSWER 2 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 145:505354 CASREACT Full-text

TITLE: Synthesis and antimicrobial activity of succinimido  
(2-aryl-4-oxo-3-[[ (quinolin-8-yloxy) acetyl] amino}-1,3-  
thiazolidin-5-yl) acetates

AUTHOR(S): Ahmed, Maqbool; Sharma, Ranjana; Nagda, Devendra P.;  
Jat, Jawahar L.; Talesara, Ganpat L.

CORPORATE SOURCE: Synthetic Organic Chemistry Laboratory, Department of  
Chemistry, M. L. Sukhadia University, Udaipur, 313  
001, India

SOURCE: ARKIVOC (Gainesville, FL, United States) (2006), (11),  
66-75

CODEN: AGFUAR

URL: [http://www.arkat-](http://www.arkat-usa.org/ark/journal/2006/I11_General/1813/06-1813BP%20as%20published%20mainmanuscript.pdf)  
[usa.org/ark/journal/2006/I11\\_General/1813/06-](http://www.arkat-usa.org/ark/journal/2006/I11_General/1813/06-1813BP%20as%20published%20mainmanuscript.pdf)  
1813BP%20as%20published%20mainmanuscript.pdf

PUBLISHER: Arkat USA Inc.

DOCUMENT TYPE: Journal; (online computer file)

LANGUAGE: English

AB 8-Hydroxyquinoline reacts with ClCH2CO2Et in the presence of anhydrous K2CO3 to produce (quinolin-8-yloxy)acetate. Subsequent treatment with N2H4.H2O forms (quinolin-8-yloxy)acetyl hydrazide, which on condensation with aromatic aldehydes gives (quinolin-8-yloxy)acetyl (1Z)-arylidenehydrazides. The latter, on cyclization with mercaptosuccinate, yield (2-aryl-4-oxo-3-[[ (quinolin-8-yloxy) acetyl] amino}-1,3-thiazolidin-5-yl) acetates. Further conversion into acid chlorides and reaction with N-hydroxysuccinimide in the presence of TEA furnishes the title compds. Antibacterial and antifungal

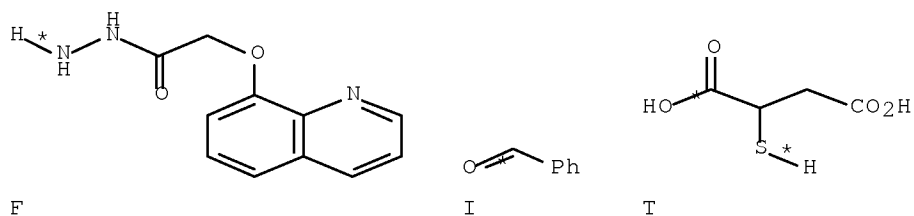
10/595943

activities of the final compds. were evaluated, and all the compds. inhibited bacterial and fungal growth.

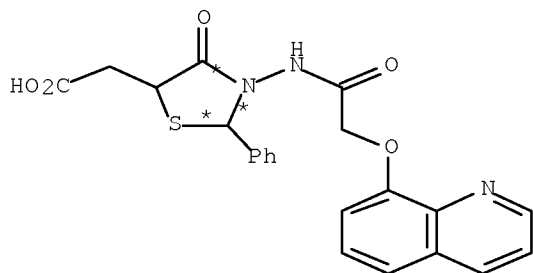
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(25) OF 69 COMPOSED OF RX(3), RX(8)

RX(25) F + I + T ==> U



2  
STEPS  
→



U  
YIELD 54%

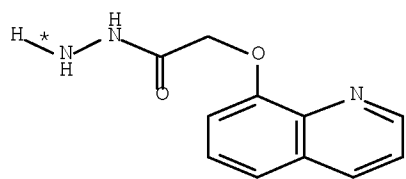
RX(3) RCT F 3281-08-1, I 100-52-7  
PRO J 42322-33-8  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 6 hours, reflux

RX(8) RCT J 42322-33-8, T 70-49-5  
PRO U 914931-89-8  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 12 - 14 hours, reflux

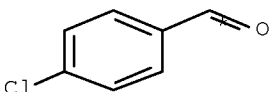
10/595943

RX(26) OF 69 COMPOSED OF RX(4), RX(9)

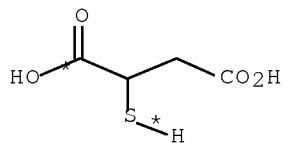
RX(26) F + L + T ==> X



F



L



T

2  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(4) RCT F 3281-08-1, L 104-88-1

PRO M 175688-48-9

CAT 64-19-7 AcOH

SOL 64-17-5 EtOH

CON 6 hours, reflux

RX(9) RCT M 175688-48-9, T 70-49-5

PRO X 914931-91-2

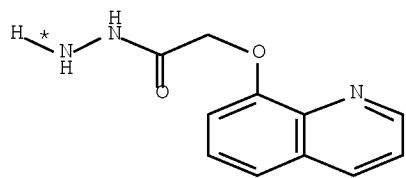
CAT 7646-85-7 ZnCl<sub>2</sub>

SOL 109-99-9 THF

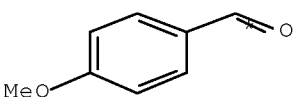
CON 12 - 14 hours, reflux

RX(27) OF 69 COMPOSED OF RX(5), RX(10)

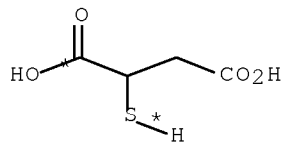
RX(27) F + N + T ==> Y



F



N



T

2  
STEPS  
→

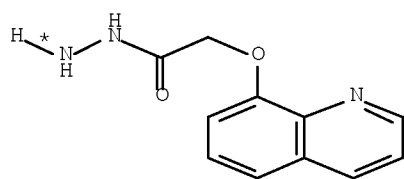
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(5) RCT F 3281-08-1, N 123-11-5  
 PRO O 59836-00-9  
 CAT 64-19-7 AcOH  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

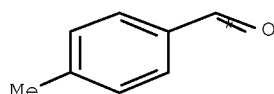
RX(10) RCT O 59836-00-9, T 70-49-5  
 PRO Y 914931-92-3  
 CAT 7646-85-7 ZnCl2  
 SOL 109-99-9 THF  
 CON 12 - 14 hours, reflux

RX(28) OF 69 COMPOSED OF RX(6), RX(11)

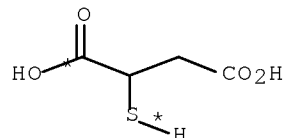
RX(28) F + P + T ==> Z



F



P



T

2  
 STEPS  
 →

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

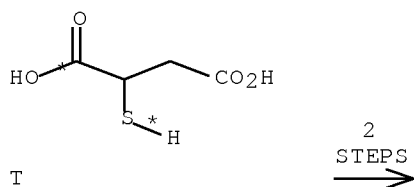
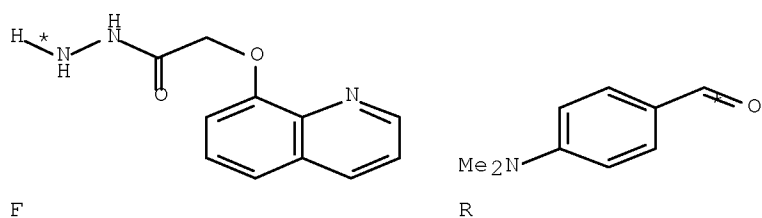
RX(6) RCT F 3281-08-1, P 104-87-0  
 PRO Q 358676-23-0  
 CAT 64-19-7 AcOH  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

RX(11) RCT Q 358676-23-0, T 70-49-5  
 PRO Z 914931-93-4  
 CAT 7646-85-7 ZnCl2  
 SOL 109-99-9 THF  
 CON 12 - 14 hours, reflux

RX(29) OF 69 COMPOSED OF RX(7), RX(12)

RX(29) F + R + T ==> AA

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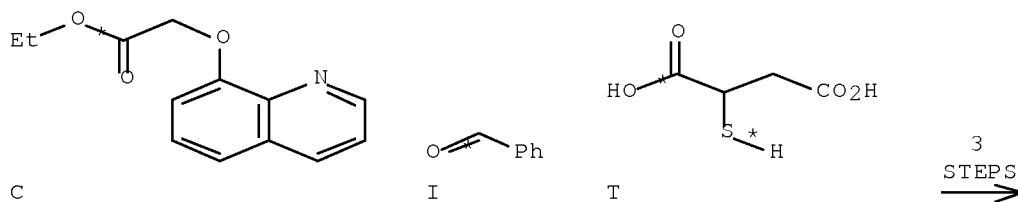
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(7)      RCT   F 3281-08-1, R 100-10-7  
              PRO   S 59836-06-5  
              CAT   64-19-7 AcOH  
              SOL   64-17-5 EtOH  
              CON   6 hours, reflux

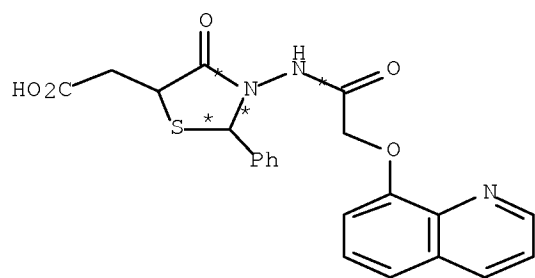
RX(12)     RCT   S 59836-06-5, T 70-49-5  
              PRO   AA 914931-94-5  
              CAT   7646-85-7 ZnCl2  
              SOL   109-99-9 THF  
              CON   12 - 14 hours, reflux

RX(41) OF 69 COMPOSED OF RX(2), RX(3), RX(8)

RX(41)      C + I + T ==> U



10/595943



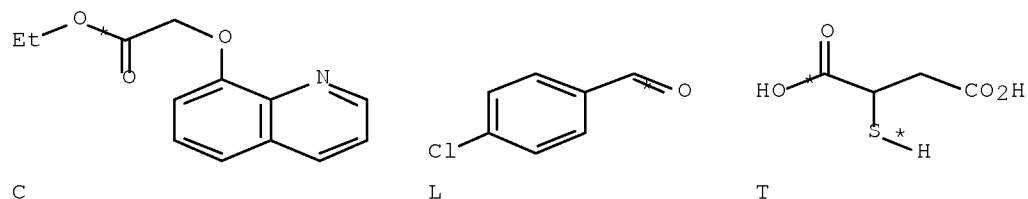
U  
YIELD 54%

RX (2) RCT C 42322-30-5  
RGT G ~~7803-57-8~~ N2H4-H2O  
PRO F 3281-08-1  
SOL 64-17-5 EtOH  
CON 6 hours, reflux

RX(3)	RCT	F 3281-08-1, I 100-52-7
	PRO	J 42322-33-8
	CAT	64-19-7 AcOH
	SOL	64-17-5 EtOH
	CON	6 hours, reflux

RX(8)            RCT   J 42322-33-8, T 70-49-5  
                 PRO   U 914931-89-8  
                 CAT   7646-85-7 ZnCl2  
                 SOL   109-99-9 THF  
                 CON   12 - 14 hours, reflux

RX(42) OF 69 COMPOSED OF RX(2), RX(4), RX(9)  
RX(42) C + L + T ==> X



3  
STEPS  
→



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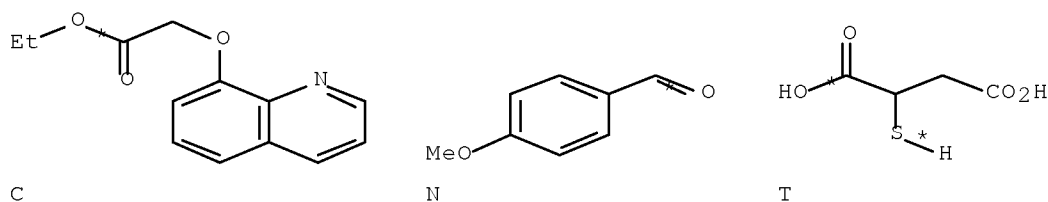
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT C 42322-30-5  
 RGT G ~~7803-57-8~~ N2H4-H2O  
 PRO F 3281-08-1  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

RX(4) RCT F 3281-08-1, L 104-88-1  
 PRO M 175688-48-9  
 CAT 64-19-7 AcOH  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

RX(9) RCT M 175688-48-9, T 70-49-5  
 PRO X 914931-91-2  
 CAT ~~7646-85-7~~ ZnCl2  
 SOL 109-99-9 THF  
 CON 12 - 14 hours, reflux

RX(43) OF 69 COMPOSED OF RX(2), RX(5), RX(10)  
 RX(43) C + N + T ==> Y



3  
 STEPS  
 →

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

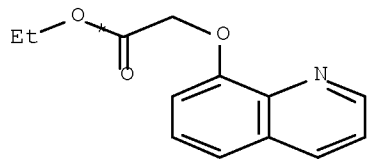
RX(2) RCT C 42322-30-5  
 RGT G ~~7803-57-8~~ N2H4-H2O  
 PRO F 3281-08-1  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

RX(5) RCT F 3281-08-1, N 123-11-5  
 PRO O 59836-00-9  
 CAT 64-19-7 AcOH  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

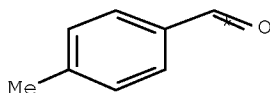
10/595943

RX(10) RCT O 59836-00-9, T 70-49-5  
 PRO Y 914931-92-3  
 CAT 7646-85-7 ZnCl2  
 SOL 109-99-9 THF  
 CON 12 - 14 hours, reflux

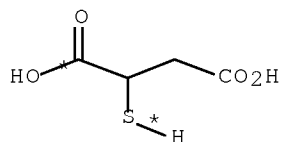
RX(44) OF 69 COMPOSED OF RX(2), RX(6), RX(11)  
 RX(44) C + P + T ==> Z



C



P



T

3  
 STEPS  
 →

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

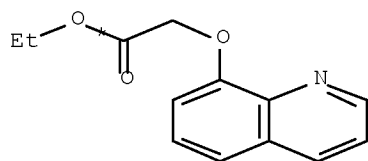
RX(2) RCT C 42322-30-5  
 RGT G 7803-57-8 N2H4-H2O  
 PRO F 3281-08-1  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

RX(6) RCT F 3281-08-1, P 104-87-0  
 PRO Q 358676-23-0  
 CAT 64-19-7 AcOH  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

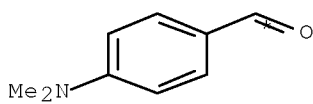
RX(11) RCT Q 358676-23-0, T 70-49-5  
 PRO Z 914931-93-4  
 CAT 7646-85-7 ZnCl2  
 SOL 109-99-9 THF  
 CON 12 - 14 hours, reflux

RX(45) OF 69 COMPOSED OF RX(2), RX(7), RX(12)  
 RX(45) C + R + T ==> AA

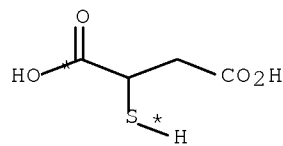
10/595943



C



R



T

3  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

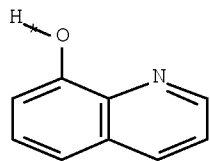
RX(2) RCT C 42322-30-5  
RGT G 7803-57-8 N2H4-H2O  
PRO F 3281-08-1  
SOL 64-17-5 EtOH  
CON 6 hours, reflux

RX(7) RCT F 3281-08-1, R 100-10-7  
PRO S 59836-06-5  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 6 hours, reflux

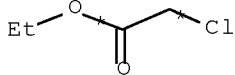
RX(12) RCT S 59836-06-5, T 70-49-5  
PRO AA 914931-94-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 12 - 14 hours, reflux

RX(46) OF 69 COMPOSED OF RX(1), RX(2), RX(3), RX(8)

RX(46) A + B + I + T ==> U



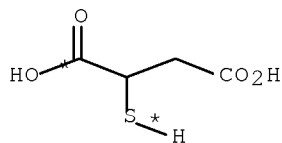
A



B



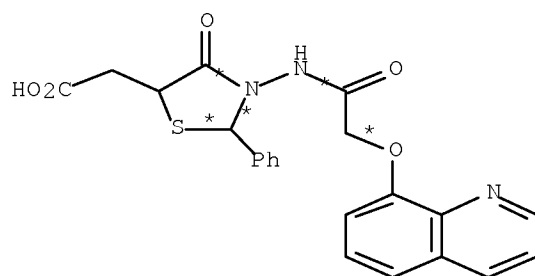
I



T

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4  
STEPS  
→



U  
YIELD 54%

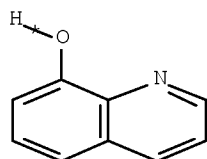
RX(1) RCT A 148-24-3, B 105-39-5  
RGT D 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO C 42322-30-5  
SOL 67-64-1 Me<sub>2</sub>CO  
CON 18 hours, reflux

RX(2) RCT C 42322-30-5  
RGT G ~~7803-57-8~~ N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
PRO F 3281-08-1  
SOL 64-17-5 EtOH  
CON 6 hours, reflux

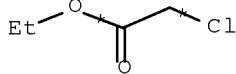
RX(3) RCT F 3281-08-1, I 100-52-7  
PRO J 42322-33-8  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 6 hours, reflux

RX(8) RCT J 42322-33-8, T ~~70-49-5~~  
PRO U ~~914931-89-8~~  
CAT ~~7546-85-7~~ ZnCl<sub>2</sub>  
SOL 109-99-9 THF  
CON 12 - 14 hours, reflux

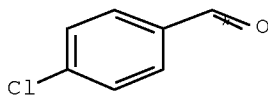
RX(47) OF 69 COMPOSED OF RX(1), RX(2), RX(4), RX(9)  
RX(47) A + B + L + T ==> X



A

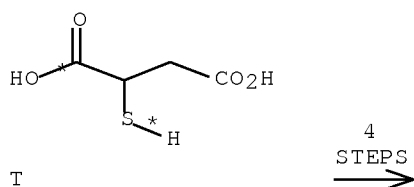


B



L

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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

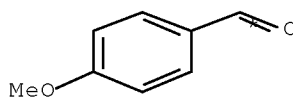
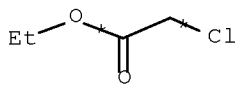
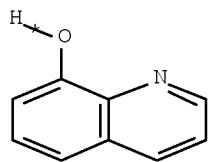
RX(1) RCT A 148-24-3, B 105-39-5  
 RGT D 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
 PRO C 42322-30-5  
 SOL 67-64-1 Me<sub>2</sub>CO  
 CON 18 hours, reflux

RX(2) RCT C 42322-30-5  
 RGT G 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
 PRO F 3281-08-1  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

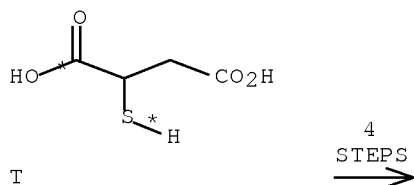
RX(4) RCT F 3281-08-1, L 104-88-1  
 PRO M 175688-48-9  
 CAT 64-19-7 AcOH  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

RX(9) RCT M 175688-48-9, T 70-49-5  
 PRO X 914931-91-2  
 CAT 7646-85-7 ZnCl<sub>2</sub>  
 SOL 109-99-9 THF  
 CON 12 - 14 hours, reflux

RX(48) OF 69 COMPOSED OF RX(1), RX(2), RX(5), RX(10)  
 RX(48) A + B + N + T ==> Y



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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

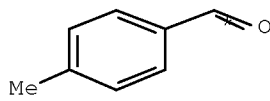
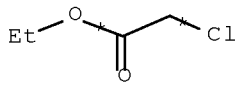
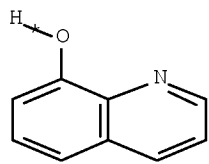
RX(1) RCT A 148-24-3, B 105-39-5  
 RGT D 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
 PRO C 42322-30-5  
 SOL 67-64-1 Me<sub>2</sub>CO  
 CON 18 hours, reflux

RX(2) RCT C 42322-30-5  
 RGT G 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
 PRO F 3281-08-1  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

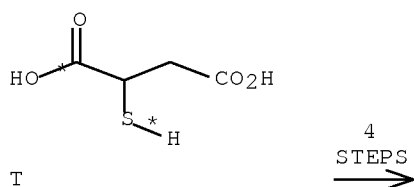
RX(5) RCT F 3281-08-1, N 123-11-5  
 PRO O 59836-00-9  
 CAT 64-19-7 AcOH  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

RX(10) RCT O 59836-00-9, T 70-49-5  
 PRO Y 914931-92-3  
 CAT 7646-85-7 ZnCl<sub>2</sub>  
 SOL 109-99-9 THF  
 CON 12 - 14 hours, reflux

RX(49) OF 69 COMPOSED OF RX(1), RX(2), RX(6), RX(11)  
 RX(49) A + B + P + T ==> Z



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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

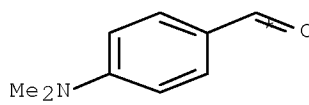
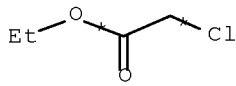
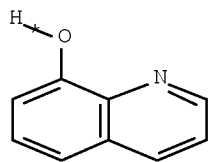
RX(1) RCT A 148-24-3, B 105-39-5  
 RGT D 584-08-7 K2CO3  
 PRO C 42322-30-5  
 SOL 67-64-1 Me2CO  
 CON 18 hours, reflux

RX(2) RCT C 42322-30-5  
 RGT G 7803-57-8 N2H4-H2O  
 PRO F 3281-08-1  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

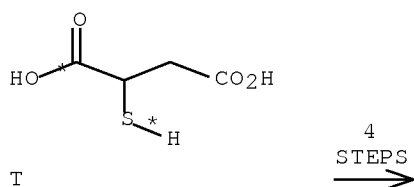
RX(6) RCT F 3281-08-1, P 104-87-0  
 PRO Q 358676-23-0  
 CAT 64-19-7 AcOH  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

RX(11) RCT Q 358676-23-0, T 70-49-5  
 PRO Z 914931-93-4  
 CAT 7646-85-7 ZnCl2  
 SOL 109-99-9 THF  
 CON 12 - 14 hours, reflux

RX(50) OF 69 COMPOSED OF RX(1), RX(2), RX(7), RX(12)  
 RX(50) A + B + R + T ==> AA



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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

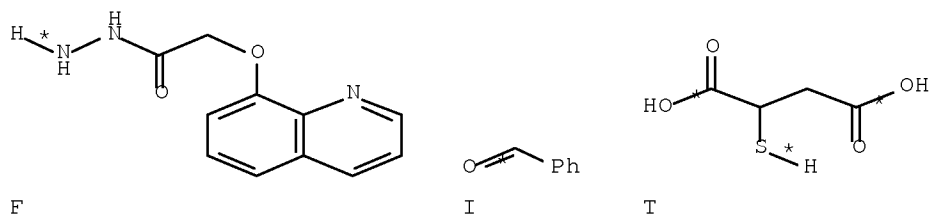
RX(1) RCT A 148-24-3, B 105-39-5  
 RGT D 584-08-7 K2CO3  
 PRO C 42322-30-5  
 SOL 67-64-1 Me2CO  
 CON 18 hours, reflux

RX(2) RCT C 42322-30-5  
 RGT G 7803-57-8 N2H4-H2O  
 PRO F 3281-08-1  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

RX(7) RCT F 3281-08-1, R 100-10-7  
 PRO S 59836-06-5  
 CAT 64-19-7 AcOH  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

RX(12) RCT S 59836-06-5, T 70-49-5  
 PRO AA 914931-94-5  
 CAT 7646-85-7 ZnCl2  
 SOL 109-99-9 THF  
 CON 12 - 14 hours, reflux

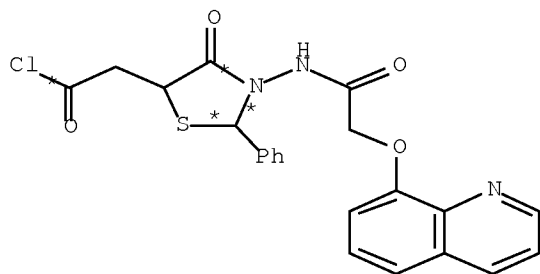
RX(51) OF 69 COMPOSED OF RX(3), RX(8), RX(13)  
 RX(51) F + I + T ==> AE



3  
STEPS  
→



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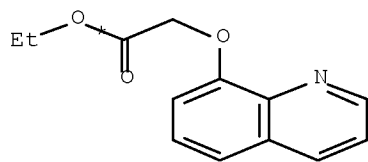
AB  
YIELD 62%

RX(3) RCT F 3281-08-1, I 100-52-7  
PRO J 42322-33-8  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 6 hours, reflux

RX(8) RCT J 42322-33-8, T 70-49-5  
PRO U 914931-89-8  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 12 - 14 hours, reflux

RX(13) RCT U 914931-89-8  
RGT AC 7719-09-7 SOCl2  
PRO AB 914931-95-6  
SOL 71-43-2 Benzene  
CON 2 - 3 hours, reflux

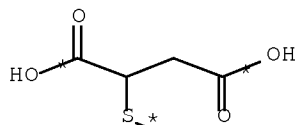
RX(52) OF 69 COMPOSED OF RX(2), RX(3), RX(8), RX(13)  
RX(52) C + I + T ==> AB



C



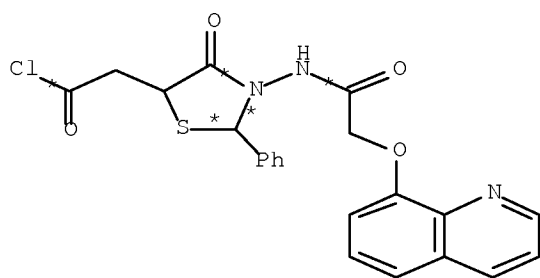
I



T

4  
STEPS  
➔

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AB  
YIELD 62%

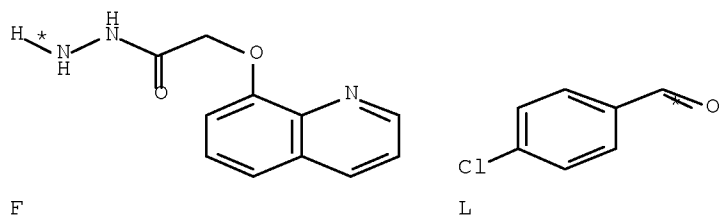
RX(2) RCT C 42322-30-5  
RGT G 7803-57-8 N2H4-H2O  
PRO F 3281-08-1  
SOL 64-17-5 EtOH  
CON 6 hours, reflux

RX(3) RCT F 3281-08-1, I 100-52-7  
PRO J 42322-33-8  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 6 hours, reflux

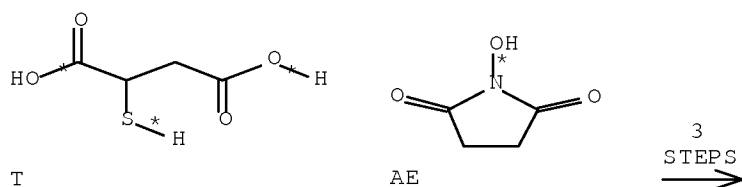
RX(8) RCT J 42322-33-8, T 70-49-5  
PRO U 914931-89-8  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 12 - 14 hours, reflux

RX(13) RCT U 914931-89-8  
RGT AC 7719-09-7 SOCl2  
PRO AB 914931-95-6  
SOL 71-43-2 Benzene  
CON 2 - 3 hours, reflux

RX(53) OF 69 COMPOSED OF RX(4), RX(9), RX(15)  
RX(53) F + L + T + AE ==> AI



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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(4) RCT F 3281-08-1, L 104-88-1  
 PRO M 175688-48-9  
 CAT 64-19-7 AcOH  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

RX(9) RCT M 175688-48-9, T 70-49-5  
 PRO X 914931-91-2  
 CAT 7646-85-7 ZnCl2  
 SOL 109-99-9 THF  
 CON 12 - 14 hours, reflux

RX(15) RCT X 914931-91-2

STAGE(1)

RGT AC 7719-09-7 SOCl2  
 SOL 71-43-2 Benzene  
 CON 2 - 3 hours, reflux

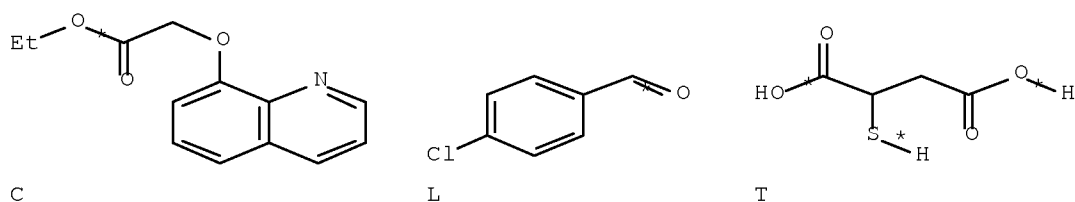
STAGE(2)

RCT AE 6066-82-6  
 RGT AG 121-44-8 Et3N  
 SOL 68-12-2 DMF  
 CON 4 - 7 hours, reflux

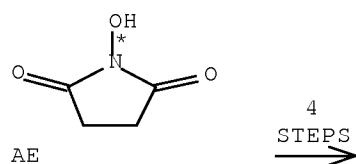
PRO AI 914931-97-8

RX(54) OF 69 COMPOSED OF RX(2), RX(4), RX(9), RX(15)

RX(54) C + L + T + AE ==> AI



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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT C 42322-30-5  
 RGT G 7803-57-8 N2H4-H2O  
 PRO F 3281-08-1  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

RX(4) RCT F 3281-08-1, L 104-88-1  
 PRO M 175688-48-9  
 CAT 64-19-7 AcOH  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

RX(9) RCT M 175688-48-9, T 70-49-5  
 PRO X 914931-91-2  
 CAT 7646-85-7 ZnCl2  
 SOL 109-99-9 THF  
 CON 12 - 14 hours, reflux

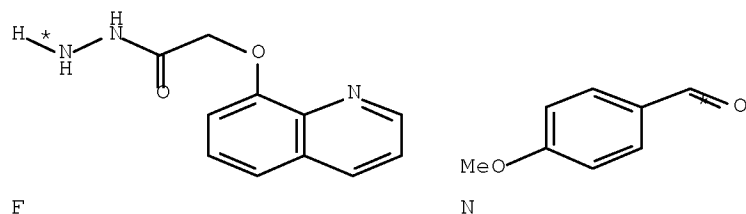
RX(15) RCT X 914931-91-2

STAGE(1)  
 RGT AC 7719-09-7 SOCl2  
 SOL 71-43-2 Benzene  
 CON 2 - 3 hours, reflux

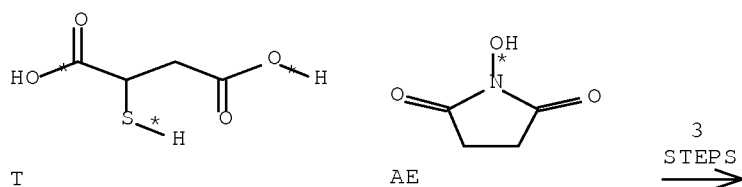
STAGE(2)  
 RCT AE 6066-82-6  
 RGT AG 121-44-8 Et3N  
 SOL 68-12-2 DMF  
 CON 4 - 7 hours, reflux

PRO AI 914931-97-8

RX(55) OF 69 COMPOSED OF RX(5), RX(10), RX(16)  
 RX(55) F + N + I + AE ==> AJ



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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(5) RCT F 3281-08-1, N 123-11-5  
 PRO O 59836-00-9  
 CAT 64-19-7 AcOH  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

RX(10) RCT O 59836-00-9, T 70-49-5  
 PRO Y 914931-92-3  
 CAT 7646-85-7 ZnCl2  
 SOL 109-99-9 THF  
 CON 12 - 14 hours, reflux

RX(16) RCT Y 914931-92-3

STAGE(1)

RGT AC 7719-09-7 SOCl2  
 SOL 71-43-2 Benzene  
 CON 2 - 3 hours, reflux

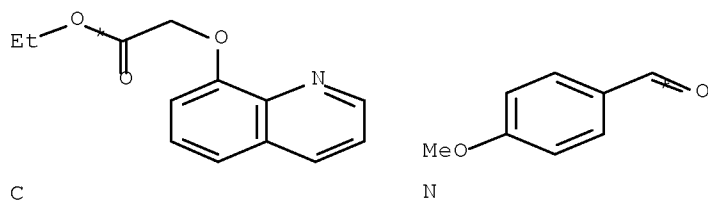
STAGE(2)

RCT AE 6066-82-6  
 RGT AG 121-44-8 Et3N  
 SOL 68-12-2 DMF  
 CON 4 - 7 hours, reflux

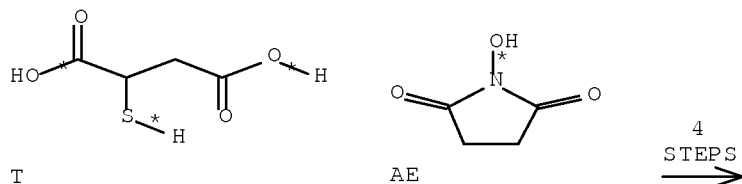
PRO AJ 914931-98-9

RX(56) OF 69 COMPOSED OF RX(2), RX(5), RX(10), RX(16)

RX(56) C + N + T + AE ==> AJ



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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

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RX(2)      RCT  C 42322-30-5
           RGT  G 7803-57-8 N2H4-H2O
           PRO  F 3281-08-1
           SOL  64-17-5 EtOH
           CON  6 hours, reflux

RX(5)      RCT  F 3281-08-1, N 123-11-5
           PRO  O 59836-00-9
           CAT  64-19-7 AcOH
           SOL  64-17-5 EtOH
           CON  6 hours, reflux

RX(10)     RCT  O 59836-00-9, T 70-49-5
           PRO  Y 914931-92-3
           CAT  7646-85-7 ZnCl2
           SOL  109-99-9 THF
           CON  12 - 14 hours, reflux

RX(16)     RCT  Y 914931-92-3

           STAGE(1)
           RGT  AC 7719-09-7 SOCl2
           SOL  71-43-2 Benzene
           CON  2 - 3 hours, reflux

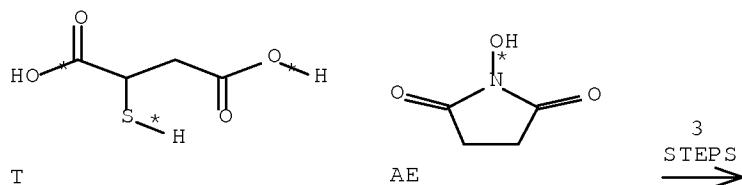
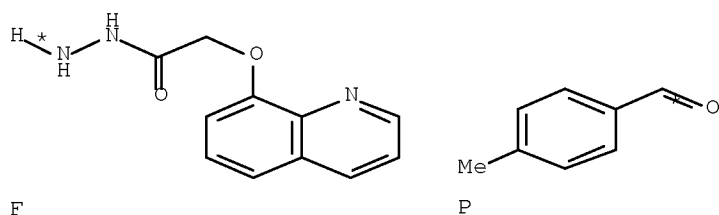
           STAGE(2)
           RCT  AE 6066-82-6
           RGT  AG 121-44-8 Et3N
           SOL  68-12-2 DMF
           CON  4 - 7 hours, reflux

           PRO  AJ 914931-98-9
  
```

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RX(57) OF 69 COMPOSED OF RX(6), RX(11), RX(17)
RX(57)    F + P + T + AE ==> AK
  
```

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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(6) RCT F 3281-08-1, P 104-87-0  
 PRO Q 358676-23-0  
 CAT 64-19-7 AcOH  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

RX(11) RCT Q 358676-23-0, T 70-49-5  
 PRO Z 914931-93-4  
 CAT 7646-85-7 ZnCl2  
 SOL 109-99-9 THF  
 CON 12 - 14 hours, reflux

RX(17) RCT Z 914931-93-4

STAGE(1)

RGT AC 7719-09-7 SOCl2  
 SOL 71-43-2 Benzene  
 CON 2 - 3 hours, reflux

STAGE(2)

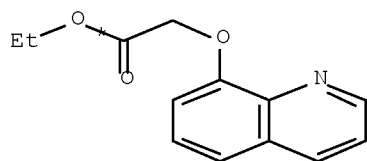
RCT AE 6066-82-6  
 RGT AG 121-44-8 Et3N  
 SOL 68-12-2 DMF  
 CON 4 - 7 hours, reflux

PRO AK 914931-99-0

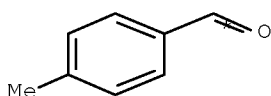
RX(58) OF 69 COMPOSED OF RX(2), RX(6), RX(11), RX(17)

RX(58) C + P + T + AE ==> AK

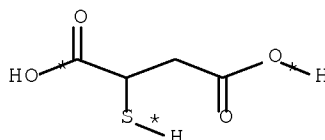
10/595943



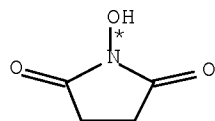
C



P



T



AE

4  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

```

RX(2)      RCT  C 42322-30-5
           RGT  G 7803-57-8 N2H4-H2O
           PRO  F 3281-08-1
           SOL  64-17-5 EtOH
           CON  6 hours, reflux

RX(6)      RCT  F 3281-08-1, P 104-87-0
           PRO  Q 358676-23-0
           CAT  64-19-7 AcOH
           SOL  64-17-5 EtOH
           CON  6 hours, reflux

RX(11)     RCT  Q 358676-23-0, T 70-49-5
           PRO  Z 914931-93-4
           CAT  7646-85-7 ZnCl2
           SOL  109-99-9 THF
           CON  12 - 14 hours, reflux

RX(17)     RCT  Z 914931-93-4

           STAGE(1)
           RGT  AC 7719-09-7 SOCl2
           SOL  71-43-2 Benzene
           CON  2 - 3 hours, reflux

           STAGE(2)
           RCT  AE 6066-82-6
           RGT  AG 121-44-8 Et3N
           SOL  68-12-2 DMF
           CON  4 - 7 hours, reflux

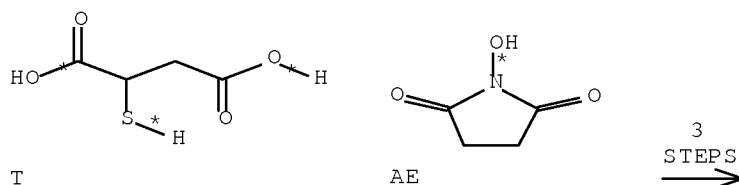
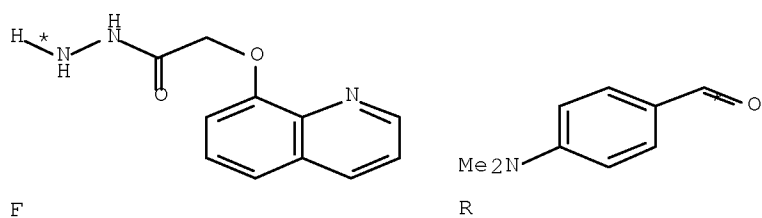
           PRO  AK 914931-99-0
  
```

RX(59) OF 69 COMPOSED OF RX(7), RX(12), RX(18)



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RX(59) F + R + T + AE ==> AL



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(7) RCT F 3281-08-1, R 100-10-7  
 PRO S 59836-06-5  
 CAT 64-19-7 AcOH  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

RX(12) RCT S 59836-06-5, T 70-49-5  
 PRO AA 914931-94-5  
 CAT ~~7546-85-7~~ ZnCl2  
 SOL 109-99-9 THF  
 CON 12 - 14 hours, reflux

RX(18) RCT AA 914931-94-5

STAGE(1)

RGT AC 7719-09-7 SOCl2  
 SOL 71-43-2 Benzene  
 CON 2 - 3 hours, reflux

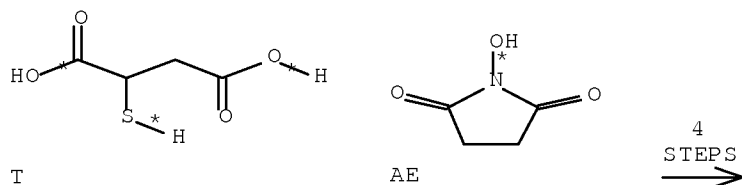
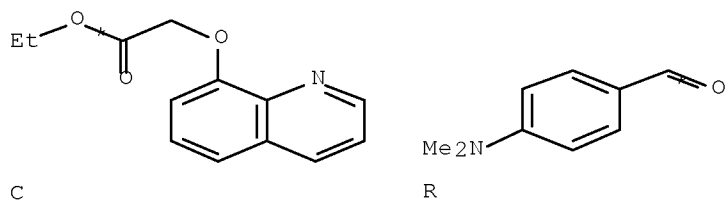
STAGE(2)

RCT AE 6066-82-6  
 RGT AG 121-44-8 Et3N  
 SOL 68-12-2 DMF  
 CON 4 - 7 hours, reflux

PRO AL 914932-00-6

RX(60) OF 69 COMPOSED OF RX(2), RX(7), RX(12), RX(18)  
 RX(60) C + R + T + AE ==> AL

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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

```

RX(2)      RCT  C 42322-30-5
           RGT  G 7803-57-8 N2H4-H2O
           PRO  F 3281-08-1
           SOL  64-17-5 EtOH
           CON  6 hours, reflux

RX(7)      RCT  F 3281-08-1, R 100-10-7
           PRO  S 59836-06-5
           CAT  64-19-7 AcOH
           SOL  64-17-5 EtOH
           CON  6 hours, reflux

RX(12)     RCT  S 59836-06-5, T 70-49-5
           PRO  AA 914931-94-5
           CAT  7646-85-7 ZnCl2
           SOL  109-99-9 THF
           CON  12 - 14 hours, reflux

RX(18)     RCT  AA 914931-94-5

           STAGE(1)
             RGT  AC 7719-09-7 SOCl2
             SOL  71-43-2 Benzene
             CON  2 - 3 hours, reflux

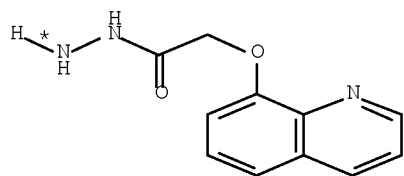
           STAGE(2)
             RCT  AE 6066-82-6
             RGT  AG 121-44-8 Et3N
             SOL  68-12-2 DMF
             CON  4 - 7 hours, reflux

           PRO  AL 914932-00-6
  
```

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RX(62) OF 69 COMPOSED OF RX(3), RX(8), RX(13), RX(14)

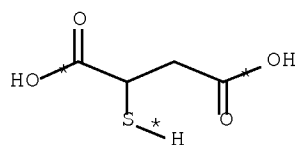
RX(62) F + I + T + AE ==> AF



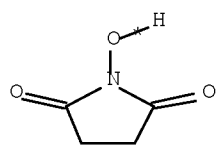
F



I

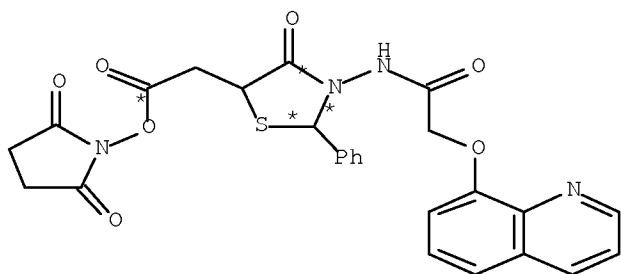


T



AE

4  
STEPS  
→



AF  
YIELD 66%

RX(3) RCT F 3281-08-1, I 100-52-7  
PRO J 42322-33-8  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 6 hours, reflux

RX(8) RCT J 42322-33-8, T 70-49-5  
PRO U 914931-89-8  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 12 - 14 hours, reflux

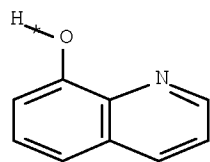
RX(13) RCT U 914931-89-8  
RGT AC 7719-09-7 SOCl2  
PRO AB 914931-95-6

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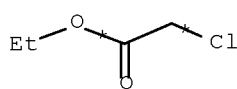
SOL 71-43-2 Benzene  
CON 2 - 3 hours, reflux

RX(14) RCT AB 914931-95-6, AE 6066-82-6  
RGT AG 121-44-8 Et3N  
PRO AF 914931-96-7  
SOL 68-12-2 DMF  
CON 4 - 7 hours, reflux

RX(63) OF 69 COMPOSED OF RX(1), RX(2), RX(3), RX(8), RX(13)  
RX(63) A + B + I + T ==> AB



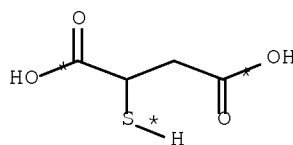
A



B

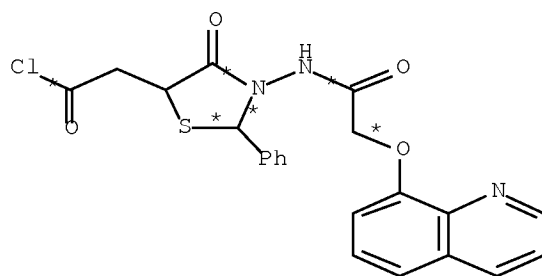


I



T

5  
STEPS  
→



AB  
YIELD 62%

RX(1) RCT A 148-24-3, B 105-39-5  
RGT D 584-08-7 K2CO3  
PRO C 42322-30-5  
SOL 67-64-1 Me2CO  
CON 18 hours, reflux

RX(2) RCT C 42322-30-5  
RGT G 7803-57-8 N2H4-H2O  
PRO F 3281-08-1  
SOL 64-17-5 EtOH  
CON 6 hours, reflux

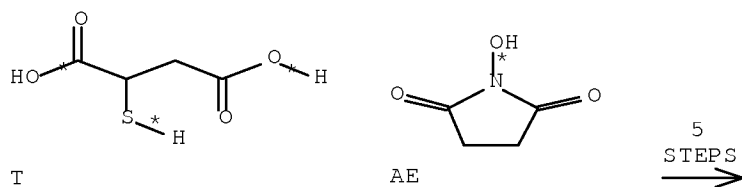
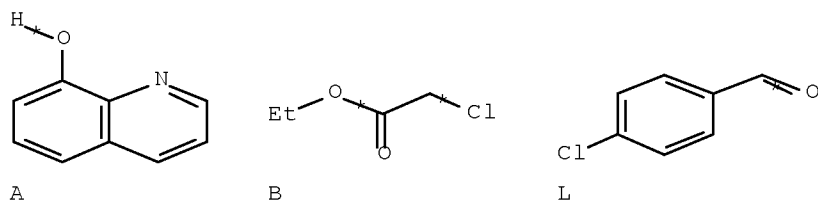
RX(3) RCT F 3281-08-1, I 100-52-7  
PRO J 42322-33-8  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 6 hours, reflux

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RX(8) RCT J 42322-33-8, T 70-49-5  
PRO U 914931-89-8  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 12 - 14 hours, reflux

RX(13) RCT U 914931-89-8  
RGT AC 7719-09-7 SOCl2  
PRO AB 914931-95-6  
SOL 71-43-2 Benzene  
CON 2 - 3 hours, reflux

RX(64) OF 69 COMPOSED OF RX(1), RX(2), RX(4), RX(9), RX(15)  
RX(64) A + B + L + T + AE ==> AI



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(1) RCT A 148-24-3, B 105-39-5  
RGT D 584-08-7 K2CO3  
PRO C 42322-30-5  
SOL 67-64-1 Me2CO  
CON 18 hours, reflux

RX(2) RCT C 42322-30-5  
RGT G 7803-57-8 N2H4-H2O  
PRO F 3281-08-1  
SOL 64-17-5 EtOH  
CON 6 hours, reflux

RX(4) RCT F 3281-08-1, L 104-88-1  
PRO M 175688-48-9  
CAT 64-19-7 AcOH

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SOL 64-17-5 EtOH  
CON 6 hours, reflux

RX(9) RCT M 175688-48-9, T 70-49-5  
PRO X 914931-91-2  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 12 - 14 hours, reflux

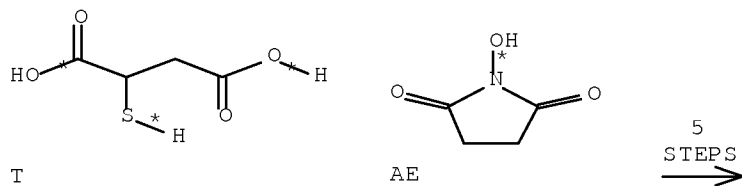
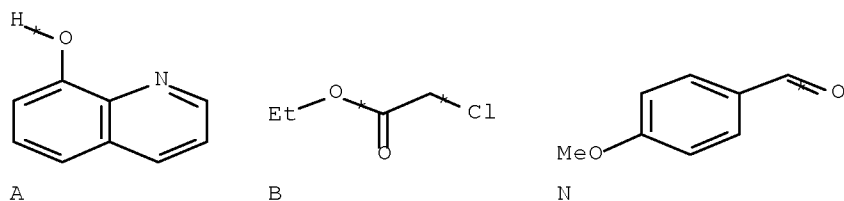
RX(15) RCT X 914931-91-2

STAGE(1)  
RGT AC 7719-09-7 SOCl2  
SOL 71-43-2 Benzene  
CON 2 - 3 hours, reflux

STAGE(2)  
RCT AE 6066-82-6  
RGT AG 121-44-8 Et3N  
SOL 68-12-2 DMF  
CON 4 - 7 hours, reflux

PRO AI 914931-97-8

RX(65) OF 69 COMPOSED OF RX(1), RX(2), RX(5), RX(10), RX(16)  
RX(65) A + B + N + T + AE ==> AJ



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(1) RCT A 148-24-3, B 105-39-5  
RGT D 584-08-7 K2CO3  
PRO C 42322-30-5  
SOL 67-64-1 Me2CO

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CON 18 hours, reflux

RX(2) RCT C 42322-30-5  
RGT G ~~7803-57-8~~ N2H4-H2O  
PRO F 3281-08-1  
SOL 64-17-5 EtOH  
CON 6 hours, reflux

RX(5) RCT F 3281-08-1, N 123-11-5  
PRO O 59836-00-9  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 6 hours, reflux

RX(10) RCT O 59836-00-9, T ~~70-49-5~~  
PRO Y 914931-92-3  
CAT ~~7646-85-7~~ ZnCl2  
SOL 109-99-9 THF  
CON 12 - 14 hours, reflux

RX(16) RCT Y 914931-92-3

STAGE(1)

RGT AC 7719-09-7 SOCl2  
SOL 71-43-2 Benzene  
CON 2 - 3 hours, reflux

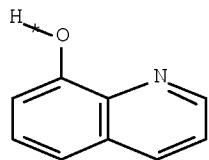
STAGE(2)

RCT AE 6066-82-6  
RGT AG 121-44-8 Et3N  
SOL 68-12-2 DMF  
CON 4 - 7 hours, reflux

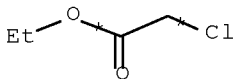
PRO AJ 914931-98-9

RX(66) OF 69 COMPOSED OF RX(1), RX(2), RX(6), RX(11), RX(17)

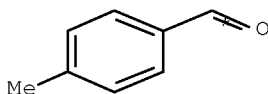
RX(66) A + B + P + T + AE ==> AK



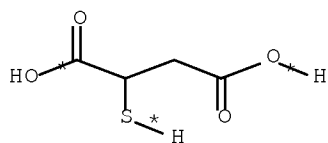
A



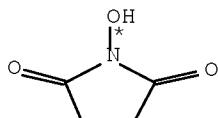
B



P



T



AE

5  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(1) RCT A 148-24-3, B 105-39-5  
 RGT D 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
 PRO C 42322-30-5  
 SOL 67-64-1 Me<sub>2</sub>CO  
 CON 18 hours, reflux

RX(2) RCT C 42322-30-5  
 RGT G ~~7803-57-8~~ N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
 PRO F 3281-08-1  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

RX(6) RCT F 3281-08-1, P 104-87-0  
 PRO Q 358676-23-0  
 CAT 64-19-7 AcOH  
 SOL 64-17-5 EtOH  
 CON 6 hours, reflux

RX(11) RCT Q 358676-23-0, T ~~70-49-5~~  
 PRO Z 914931-93-4  
 CAT ~~7646-85-7~~ ZnCl<sub>2</sub>  
 SOL 109-99-9 THF  
 CON 12 - 14 hours, reflux

RX(17) RCT Z 914931-93-4

## STAGE(1)

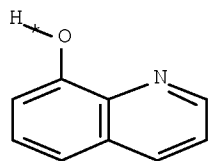
RGT AC 7719-09-7 SOCl<sub>2</sub>  
 SOL 71-43-2 Benzene  
 CON 2 - 3 hours, reflux

## STAGE(2)

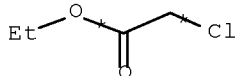
RCT AE 6066-82-6  
 RGT AG 121-44-8 Et<sub>3</sub>N  
 SOL 68-12-2 DMF  
 CON 4 - 7 hours, reflux

PRO AK 914931-99-0

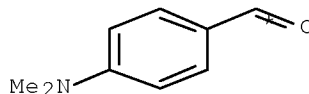
RX(67) OF 69 COMPOSED OF RX(1), RX(2), RX(7), RX(12), RX(18)  
 RX(67) A + B + R + T + AE ==> AL



A

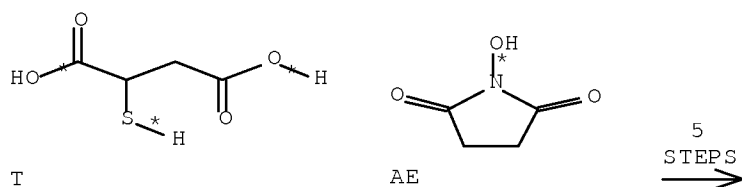


B



R





\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(1)      RCT    A 148-24-3, B 105-39-5  
              RGT    D 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
              PRO    C 42322-30-5  
              SOL    67-64-1 Me<sub>2</sub>CO  
              CON    18 hours, reflux

RX(2)      RCT    C 42322-30-5  
              RGT    G ~~7803-57-8~~ N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
              PRO    F 3281-08-1  
              SOL    64-17-5 EtOH  
              CON    6 hours, reflux

RX(7)      RCT    F 3281-08-1, R 100-10-7  
              PRO    S 59836-06-5  
              CAT    64-19-7 AcOH  
              SOL    64-17-5 EtOH  
              CON    6 hours, reflux

RX(12)     RCT    S 59836-06-5, T ~~70-49-5~~  
              PRO    AA 914931-94-5  
              CAT    ~~7646-85-7~~ ZnCl<sub>2</sub>  
              SOL    109-99-9 THF  
              CON    12 - 14 hours, reflux

RX(18)     RCT    AA 914931-94-5

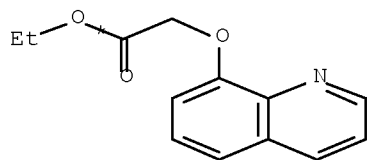
STAGE(1)  
              RGT    AC 7719-09-7 SOCl<sub>2</sub>  
              SOL    71-43-2 Benzene  
              CON    2 - 3 hours, reflux

STAGE(2)  
              RCT    AE 6066-82-6  
              RGT    AG 121-44-8 Et<sub>3</sub>N  
              SOL    68-12-2 DMF  
              CON    4 - 7 hours, reflux

PRO    AL 914932-00-6

RX(68) OF 69 COMPOSED OF RX(2), RX(3), RX(8), RX(13), RX(14)  
 RX(68)      C + I + T + AE ==> AF

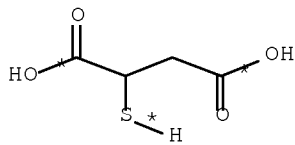
10/595943



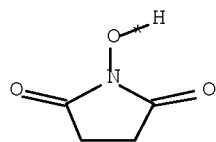
C



I

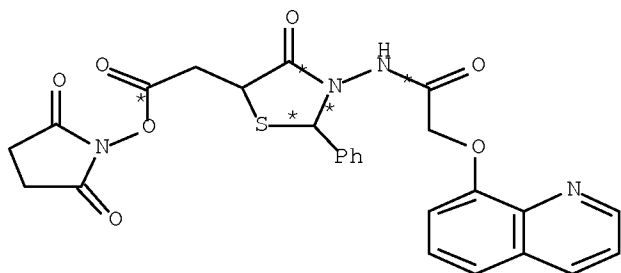


T



AE

5  
STEPS  
→



AF  
YIELD 66%

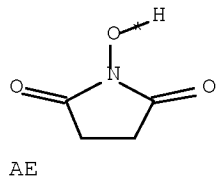
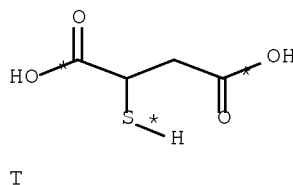
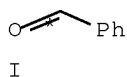
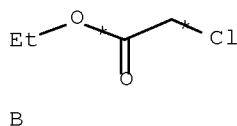
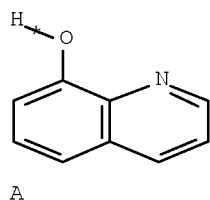
RX(2)	RCT	C 42322-30-5
	RGT	G 7803-57-8 N2H4-H2O
	PRO	F 3281-08-1
	SOL	64-17-5 EtOH
	CON	6 hours, reflux
RX(3)	RCT	F 3281-08-1, I 100-52-7
	PRO	J 42322-33-8
	CAT	64-19-7 AcOH
	SOL	64-17-5 EtOH
	CON	6 hours, reflux
RX(8)	RCT	J 42322-33-8, T 70-49-5
	PRO	U 914931-89-8
	CAT	7646-85-7 ZnCl2
	SOL	109-99-9 THF
	CON	12 - 14 hours, reflux

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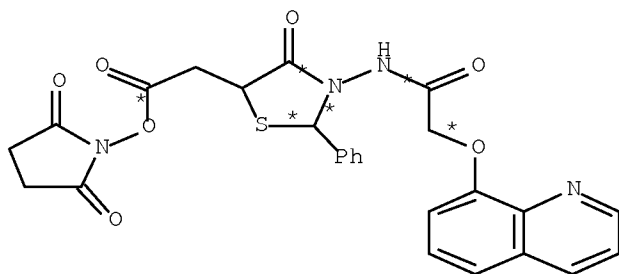
RX(13) RCT U 914931-89-8  
 RGT AC 7719-09-7 SOCl<sub>2</sub>  
 PRO AB 914931-95-6  
 SOL 71-43-2 Benzene  
 CON 2 - 3 hours, reflux

RX(14) RCT AB 914931-95-6, AE 6066-82-6  
 RGT AG 121-44-8 Et<sub>3</sub>N  
 PRO AF 914931-96-7  
 SOL 68-12-2 DMF  
 CON 4 - 7 hours, reflux

RX(69) OF 69 COMPOSED OF RX(1), RX(2), RX(3), RX(8), RX(13), RX(14)  
 RX(69) A + B + I + T + AE ==> AF



6  
 STEPS  
 ➔



AF  
 YIELD 66%

RX(1) RCT A 148-24-3, B 105-39-5  
 RGT D 584-08-7 K<sub>2</sub>CO<sub>3</sub>

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PRO C 42322-30-5  
SOL 67-64-1 Me2CO  
CON 18 hours, reflux

RX(2) RCT C 42322-30-5  
RGT G ~~7803-57-8~~ N2H4-H2O  
PRO F 3281-08-1  
SOL 64-17-5 EtOH  
CON 6 hours, reflux

RX(3) RCT F 3281-08-1, I 100-52-7  
PRO J 42322-33-8  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 6 hours, reflux

RX(8) RCT J 42322-33-8, T ~~70-49-5~~  
PRO U 914931-89-8  
CAT ~~7646-85-7~~ ZnCl2  
SOL 109-99-9 THF  
CON 12 - 14 hours, reflux

RX(13) RCT U 914931-89-8  
RGT AC 7719-09-7 SOCl2  
PRO AB 914931-95-6  
SOL 71-43-2 Benzene  
CON 2 - 3 hours, reflux

RX(14) RCT AB 914931-95-6, AE 6066-82-6  
RGT AG 121-44-8 Et3N  
PRO AF ~~914931-96-7~~  
SOL 68-12-2 DMF  
CON 4 - 7 hours, reflux

L91 ANSWER 3 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 145:188600 CASREACT Full-text

TITLE: Synthesis of phthalimido/succinimido [2-substituted  
aryl-3-(N7-theophyllinylacetamidyl)-4-oxo-1,3-  
thiazolidin-5-yl]ethanoic acids

AUTHOR(S): Sharma, Ranjana; Ahmed, Maqbool; Talesara, G. L.

CORPORATE SOURCE: Synthetic Organic Chemistry Laboratory, Department of  
Chemistry, Mohan Lal Sukhadia University, Udaipur, 313  
001, India

SOURCE: Indian Journal of Heterocyclic Chemistry (2005),  
15(1), 35-38

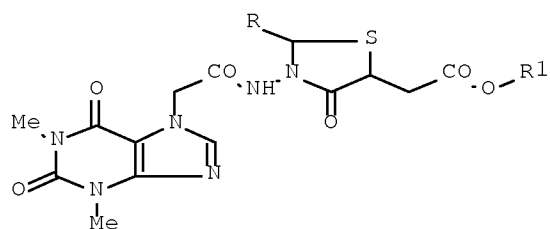
CODEN: IJCHEI; ISSN: 0971-1627

PUBLISHER: Prof. R. S. Varma

DOCUMENT TYPE: Journal

LANGUAGE: English

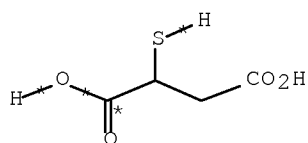
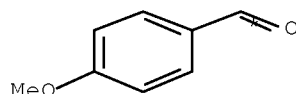
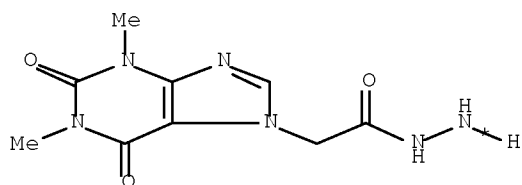
GI



AB The title theophylline derivs. I [R = Ph, C<sub>6</sub>H<sub>4</sub>-4-OMe, -4-Cl, -3-NO<sub>2</sub>, -4-NO<sub>2</sub>, -4-NMe<sub>2</sub>, C<sub>6</sub>H<sub>2</sub>-3,4,5-(OMe)<sub>3</sub>, 2-furanyl; R<sub>1</sub> = phthalimido, succinimido] were prepared via reactions of Et N<sup>7</sup>-theophyllinyl acetate with hydrazine hydrate gives N<sup>7</sup>-theophyllinylacetyl hydrazide, which on condensation with various aromatic aldehydes, RCHO, afforded the corresponding arylidene derivs. A series of 2-substituted aryl-3-(N<sup>7</sup>-theophyllinylacetamidyl)-4-oxo-1,3-thiazolidin-5-yl ethanoic acids I (R<sub>1</sub> = H) were synthesized via cycloaddn. of the arylidene derivs. with mercaptosuccinic acid. The ethanoic acids were subsequently converted into the corresponding acid chlorides, which were in turn condensed with N-hydroxyphthalimide or N-hydroxysuccinimide to furnish title compds.

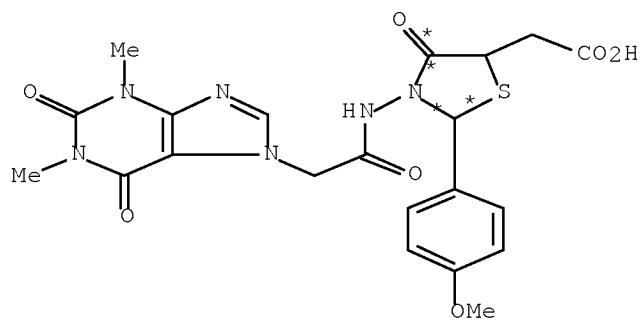
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(3) OF 139 ...F + I + J ==> K...



(3) →

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K  
YIELD 60%

RX(3) RCT F 41838-25-9, I 123-11-5

STAGE(1)

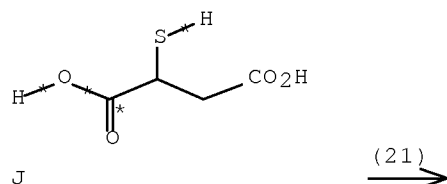
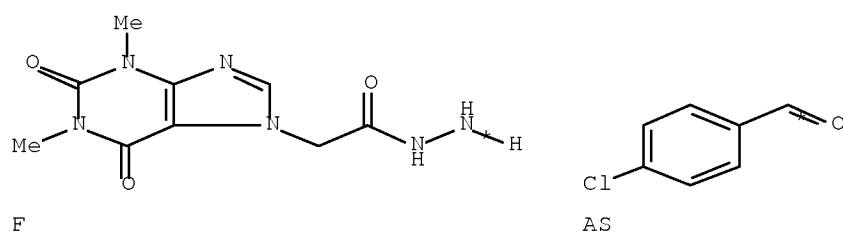
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

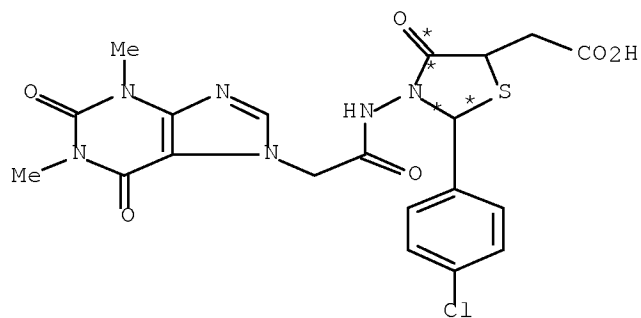
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO K 901781-44-0  
NTE intermediate was isolated

RX(21) OF 139 ...F + AS + J ==> AT...



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RX(21) RCT F 41838-25-9, AS 104-88-1

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

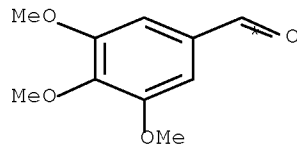
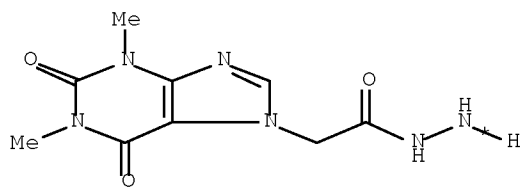
STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl<sub>2</sub>  
SOL 109-99-9 THF  
CON 10 hours, reflux

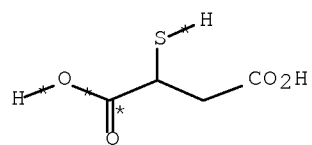
PRO AT 901781-62-2

NTE intermediate was isolated

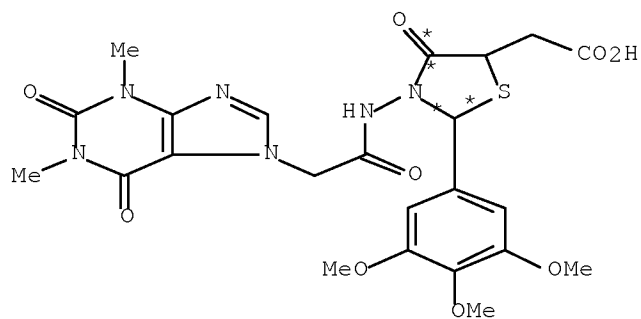
RX(22) OF 139 ...F + AU + J ==> AV...



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J



AV  
YIELD 63%

RX(22) RCT F 41838-25-9, AU 86-81-7

STAGE ( 1 )

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

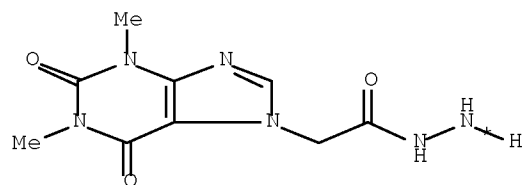
STAGE (2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

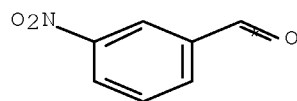
PRO AV 901781-63-3

NTE intermediate was isolated

RX(23) OF 139      ...F + AW + J ==> AX...



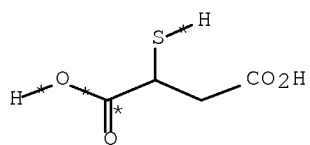
F



AW

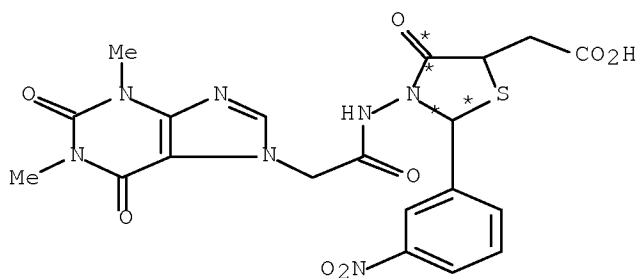


10/595943



J

(23) →



AX  
YIELD 67%

RX(23) RCT F 41838-25-9, AW 99-61-6

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

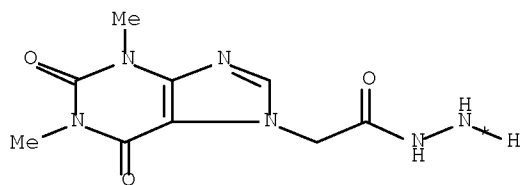
STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

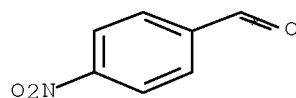
PRO AX 901781-64-4  
NTE intermediate was isolated

RX(24) OF 139 ...F + AY + J ==> AZ...

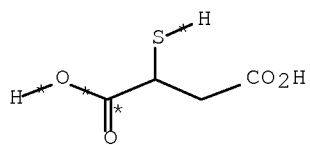
10/595943



F

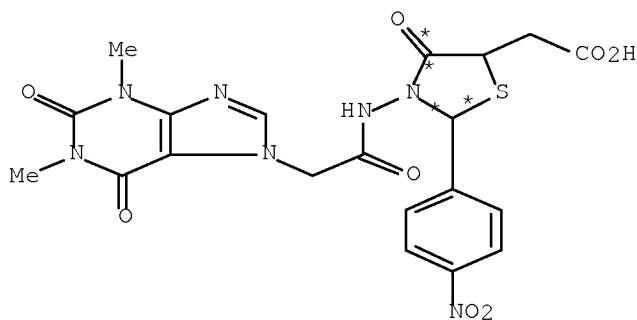


AY



J

(24)



AZ  
YIELD 61%

RX(24) RCT F 41838-25-9, AY 555-16-8

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

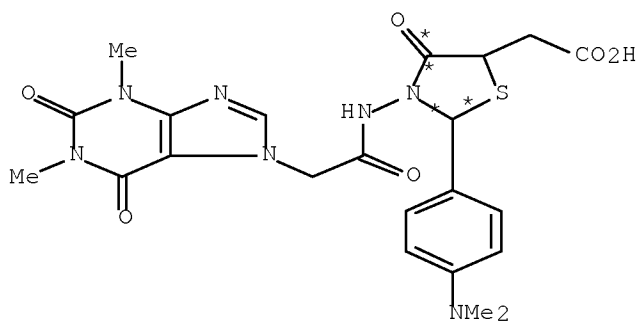
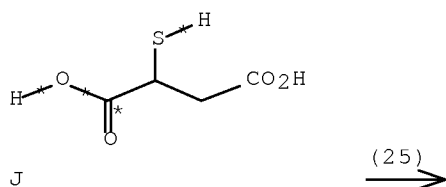
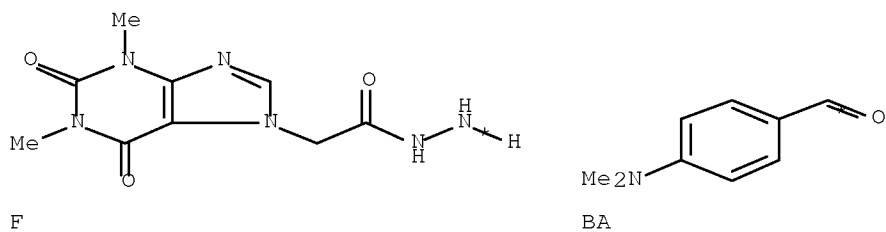
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO AZ 901781-65-5

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NTE intermediate was isolated

RX(25) OF 139 ...F + BA + J ==> BB...



YIELD 57%

RX(25) RCT F 41838-25-9, BA 100-10-7

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

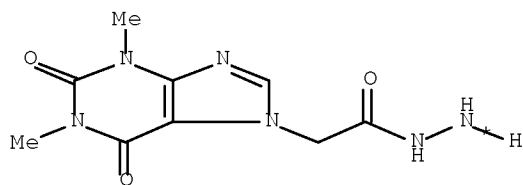
RCT J 70-49-5

10/595943

CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO BB 901781-66-6  
NTE intermediate was isolated

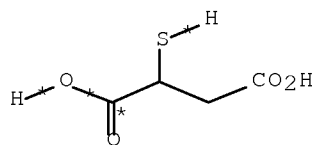
RX(26) OF 139 ...F + BC + J ==> BD...



F

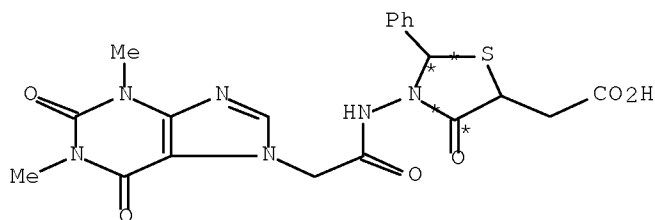


BC



J

(26)  
→



BD  
YIELD 70%

RX(26) RCT F 41838-25-9, BC 100-52-7

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

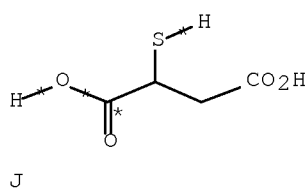
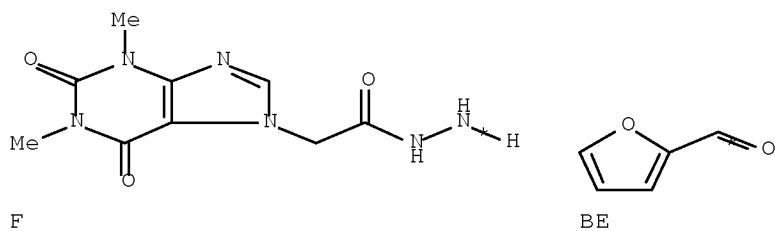
STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

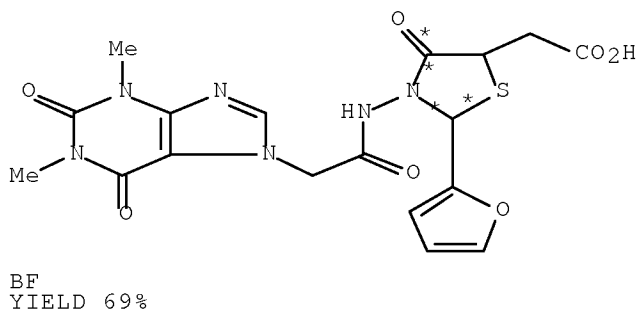
PRO BD 901781-67-7  
NTE intermediate was isolated

10/595943

RX(27) OF 139 ...F + BE + J ==> BF...



(27)



RX(27) RCT F 41838-25-9, BE 98-01-1

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

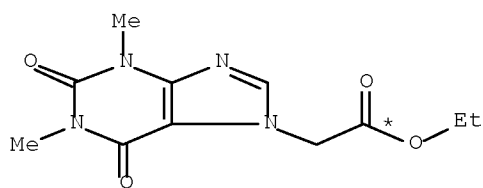
PRO BF 901781-68-8

10/595943

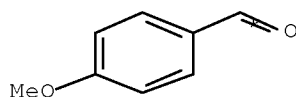
NTE intermediate was isolated

RX(36) OF 139 COMPOSED OF RX(2), RX(3)

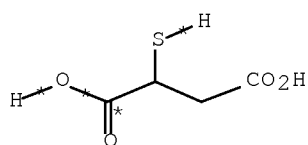
RX(36) C + I + J ==> K



C

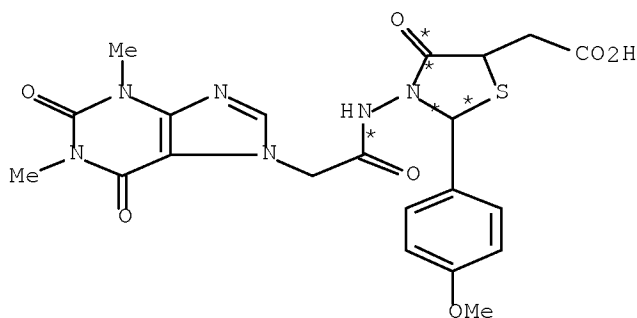


I



J

2  
STEPS  
→



K  
YIELD 60%

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(3) RCT F 41838-25-9, I 123-11-5

STAGE(1)

10/595943

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

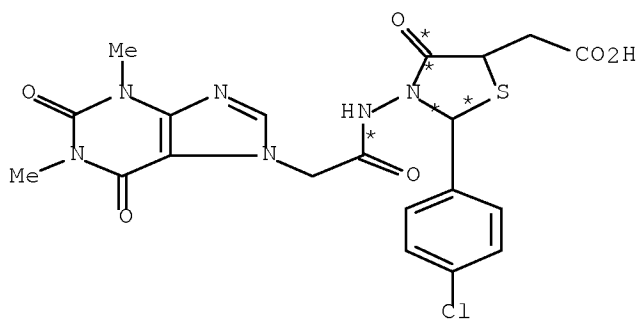
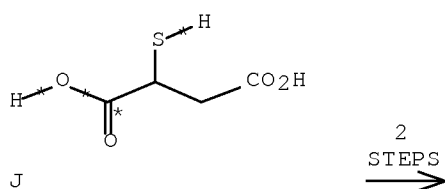
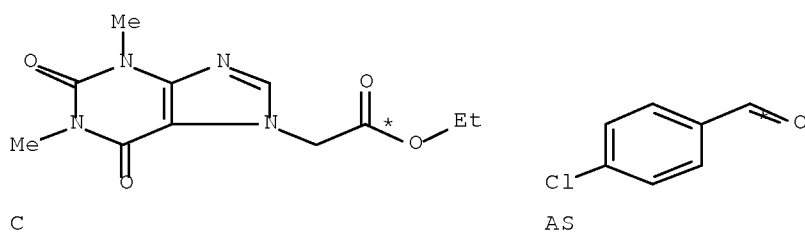
STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO K 901781-44-0  
NTE intermediate was isolated

RX(37) OF 139 COMPOSED OF RX(2), RX(21)

RX(37) C + AS + J ==> AT



YIELD 59%

10/595943

RX(2)        RCT   C 7029-96-1  
              RGT   G ~~7803-57-8~~ N2H4-H2O  
              PRO   F 41838-25-9  
              SOL   123-91-1 Dioxane  
              CON   6 hours, reflux

RX(21)      RCT   F 41838-25-9, AS 104-88-1

              STAGE(1)

                 CAT   64-19-7 AcOH  
                 SOL   64-17-5 EtOH  
                 CON   5 hours, reflux

              STAGE(2)

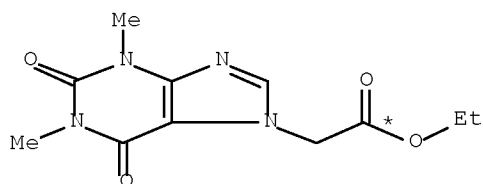
                 RCT   J ~~70-49-5~~  
                 CAT   ~~7646-85-7~~ ZnCl2  
                 SOL   109-99-9 THF  
                 CON   10 hours, reflux

              PRO   AT 901781-62-2

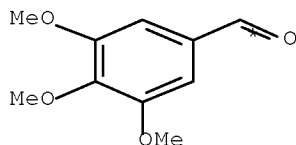
              NTE   intermediate was isolated

RX(38) OF 139 COMPOSED OF RX(2), RX(22)

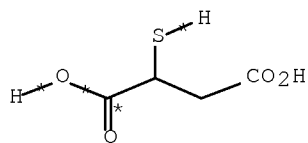
RX(38)      C + AU + J ==> AV



C



AU

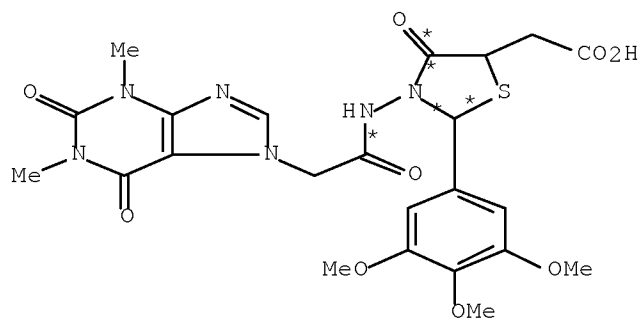


J

2  
STEPS  
→



10/595943



AV  
YIELD 63%

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

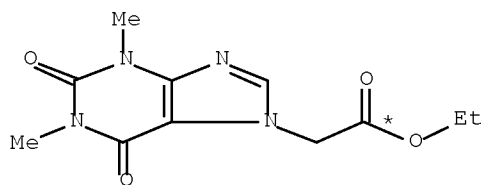
RX(22) RCT F 41838-25-9, AU 86-81-7

STAGE(1)  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

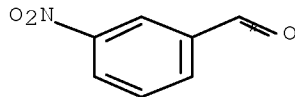
STAGE(2)  
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO AV 901781-63-3  
NTE intermediate was isolated

RX(39) OF 139 COMPOSED OF RX(2), RX(23)  
RX(39) C + AW + J ==> AX

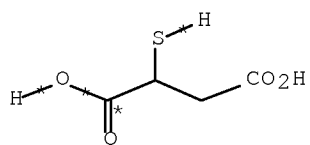


C



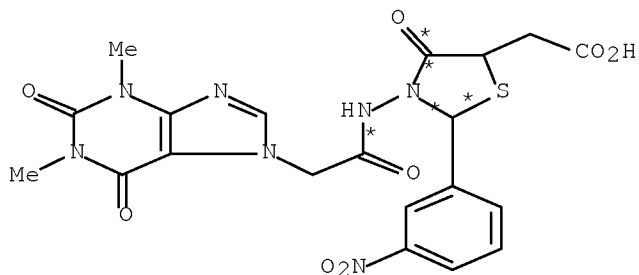
AW

10/595943



J

2  
STEPS  
→



AX  
YIELD 67%

RX(2)      RCT   C 7029-96-1  
             RGT   G 7803-57-8 N2H4-H2O  
             PRO   F 41838-25-9  
             SOL   123-91-1 Dioxane  
             CON   6 hours, reflux

RX(23)     RCT   F 41838-25-9, AW 99-61-6

STAGE(1)

CAT   64-19-7 AcOH  
SOL   64-17-5 EtOH  
CON   5 hours, reflux

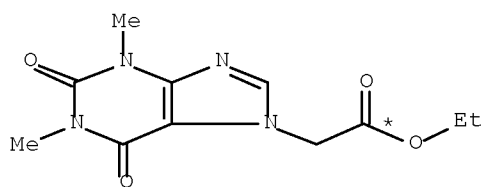
STAGE(2)

RCT   J 70-49-5  
CAT   7646-85-7 ZnCl2  
SOL   109-99-9 THF  
CON   10 hours, reflux

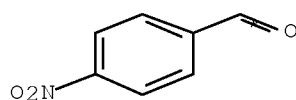
PRO   AX 901781-64-4  
NTE   intermediate was isolated

RX(40) OF 139 COMPOSED OF RX(2), RX(24)  
RX(40)      C + AY + J ==> AZ

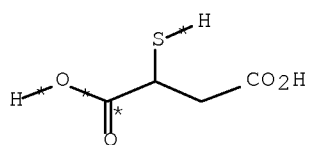
10/595943



C

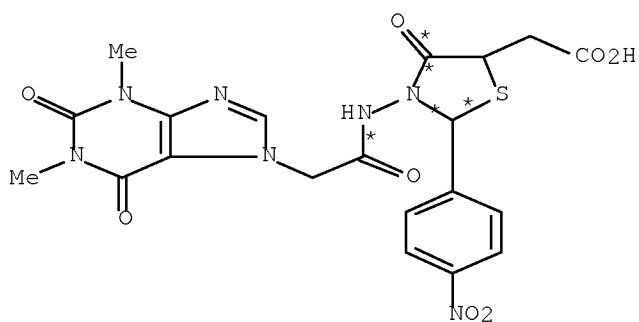


AY



J

2  
STEPS  
→



AZ  
YIELD 61%

RX(2)            RCT   C 7029-96-1  
                  RGT   G ~~7803-57-8~~ N2H4-H2O  
                  PRO   F 41838-25-9  
                  SOL   123-91-1 Dioxane  
                  CON   6 hours, reflux

RX(24) RCT F 41838-25-9, AY 555-16-8

STAGE (1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

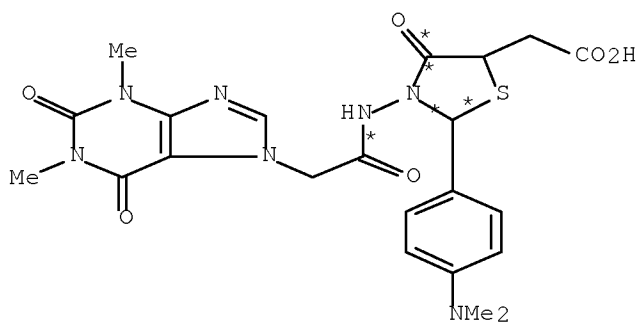
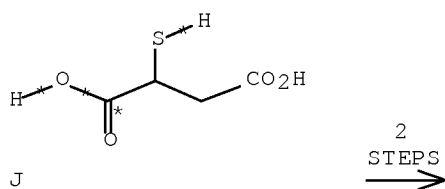
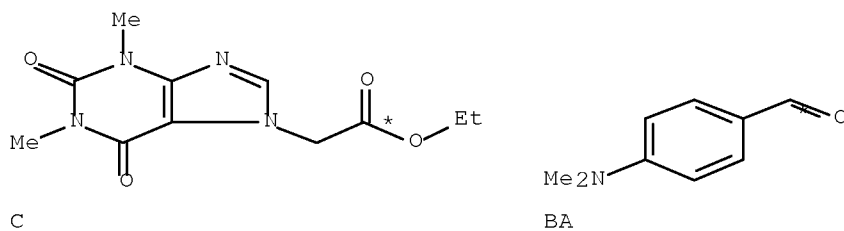
STAGE (2)

10/595943

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO AZ 901781-65-5  
NTE intermediate was isolated

RX(41) OF 139 COMPOSED OF RX(2), RX(25)  
RX(41) C + BA + J ==> BB



BB  
YIELD 57%

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O

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PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(25) RCT F 41838-25-9, BA 100-10-7

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

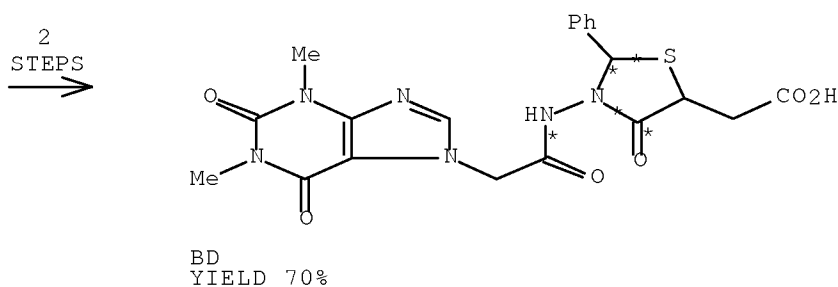
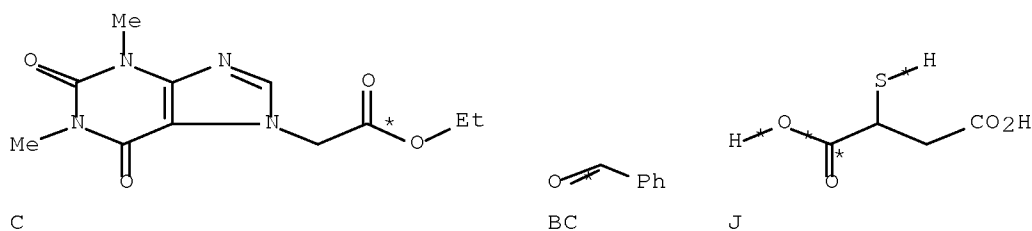
STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO BB 901781-66-6  
NTE intermediate was isolated

RX(42) OF 139 COMPOSED OF RX(2), RX(26)

RX(42) C + BC + J ==> BD



RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(26) RCT F 41838-25-9, BC 100-52-7

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STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

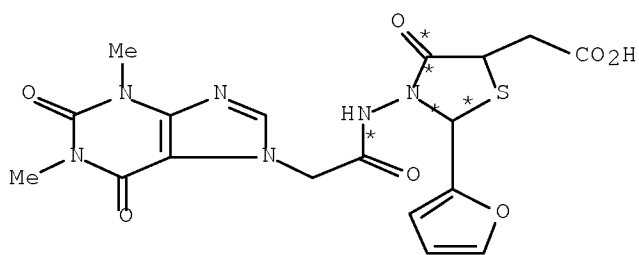
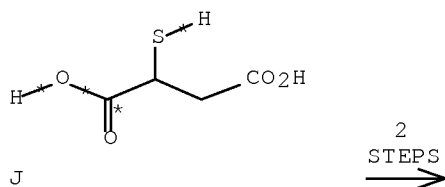
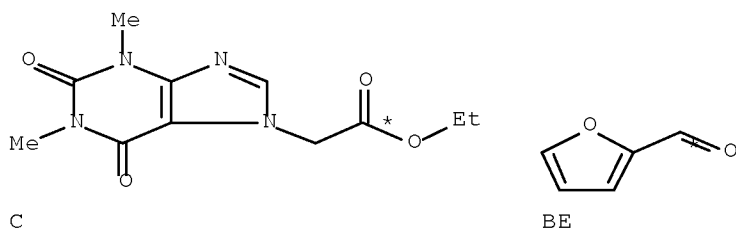
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO BD 901781-67-7

NTE intermediate was isolated

RX(43) OF 139 COMPOSED OF RX(2), RX(27)

RX(43) C + BE + J ==> BF



YIELD 69%

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RX(2)      RCT   C 7029-96-1  
            RGT   G ~~7803-57-8~~ N2H4-H2O  
            PRO   F 41838-25-9  
            SOL   123-91-1 Dioxane  
            CON   6 hours, reflux

RX(27)     RCT   F 41838-25-9, BE 98-01-1

            STAGE(1)

                CAT   64-19-7 AcOH  
                SOL   64-17-5 EtOH  
                CON   5 hours, reflux

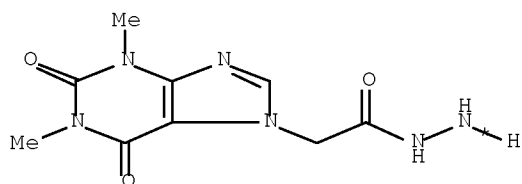
            STAGE(2)

                RCT   J ~~70-49-5~~  
                CAT   ~~7646-85-7~~ ZnCl2  
                SOL   109-99-9 THF  
                CON   10 hours, reflux

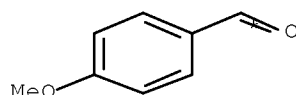
            PRO   BF 901781-68-8  
            NTE   intermediate was isolated

RX(44) OF 139 COMPOSED OF RX(3), RX(4)

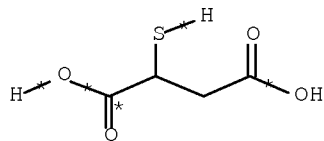
RX(44)      F + I + J ==> P



F



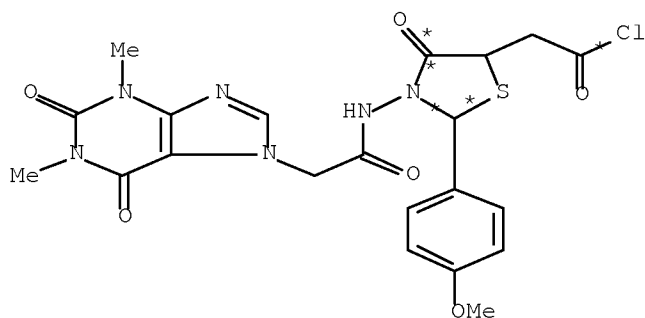
I



J

2  
STEPS  
→

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P  
YIELD 43%

RX(3) RCT F 41838-25-9, I 123-11-5

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

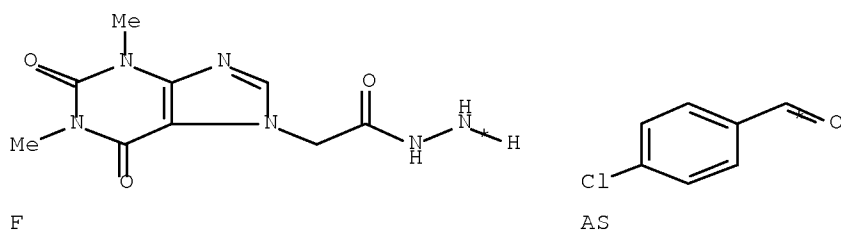
RCT J 70-49-5  
CAT 7646-85-7 ZnCl<sub>2</sub>  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO K 901781-44-0  
NTE intermediate was isolated

RX(4) RCT K 901781-44-0  
RGT Q 7719-09-7 SOCl<sub>2</sub>  
PRO P 901781-45-1  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

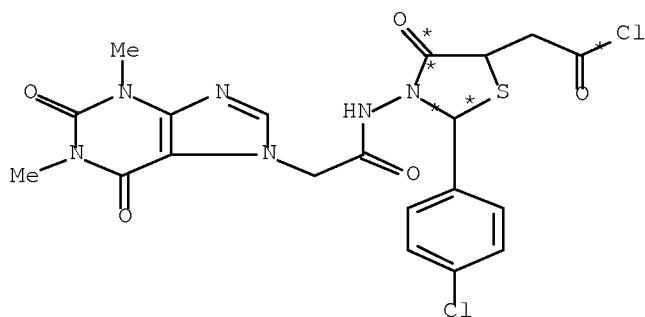
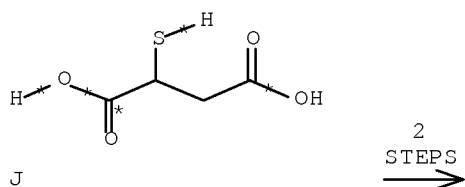
RX(47) OF 139 COMPOSED OF RX(21), RX(28)

RX(47) F + AS + J ==> V





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V  
YIELD 52%

RX(21) RCT F 41838-25-9, AS 104-88-1

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

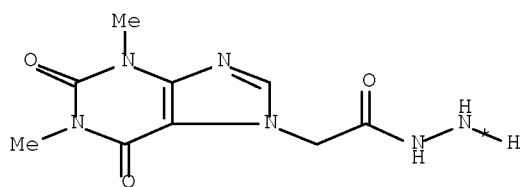
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO AT 901781-62-2  
NTE intermediate was isolated

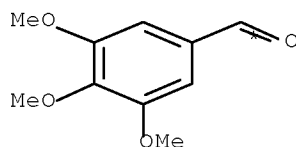
RX(28) RCT AT 901781-62-2  
RGT Q 7719-09-7 SOCl2  
PRO V 901781-69-9  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(48) OF 139 COMPOSED OF RX(22), RX(29)  
RX(48) F + AU + J ==> X

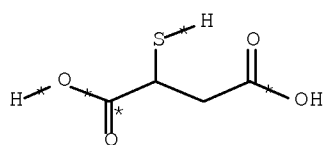
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F

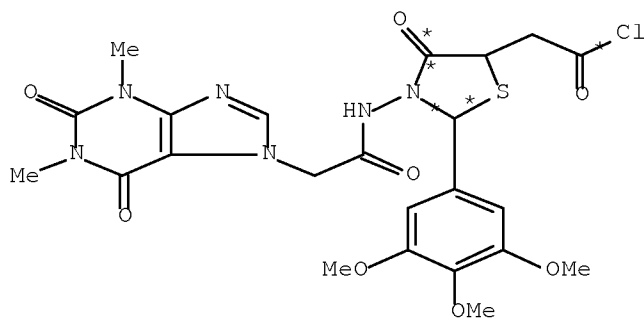


AU



J

2  
STEPS  
→



X  
YIELD 47%

RX(22) RCT F 41838-25-9, AU 86-81-7

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

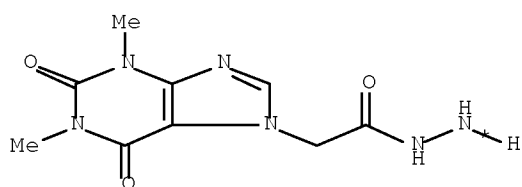
PRO AV 901781-63-3  
NTE intermediate was isolated

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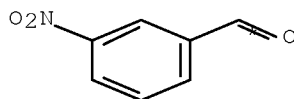
RX(29)     RCT   AV 901781-63-3  
             RGT   Q 7719-09-7 SOCl2  
             PRO   X 901781-70-2  
             SOL   108-88-3 PhMe  
             CON   30 minutes, reflux

RX(49) OF 139 COMPOSED OF RX(23), RX(30)

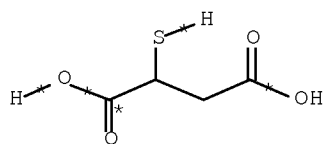
RX(49)     F + AW + J ==> Z



F

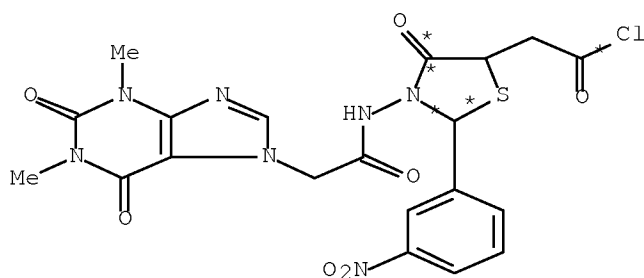


AW



J

2  
STEPS  
➔



Z  
YIELD 45%

RX(23)     RCT   F 41838-25-9, AW 99-61-6

STAGE(1)

CAT   64-19-7 AcOH

SOL   64-17-5 EtOH

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CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5

CAT 7646-85-7 ZnCl2

SOL 109-99-9 THF

CON 10 hours, reflux

PRO AX 901781-64-4

NTE intermediate was isolated

RX(30) RCT AX 901781-64-4

RGT Q 7719-09-7 SOCl2

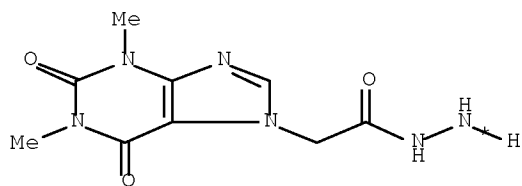
PRO Z 901781-71-3

SOL 108-88-3 PhMe

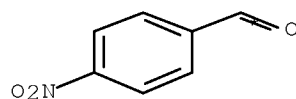
CON 30 minutes, reflux

RX(50) OF 139 COMPOSED OF RX(24), RX(31)

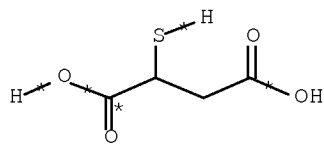
RX(50) F + AY + J ==> AB



F



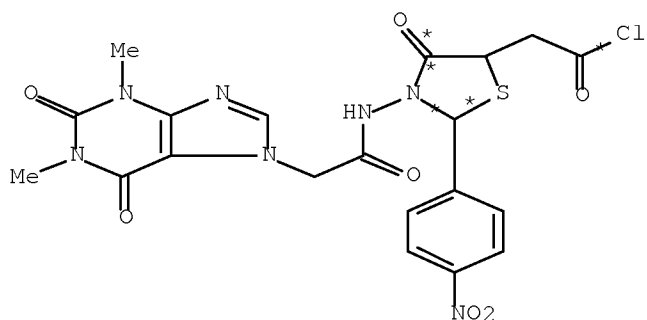
AY



J

2  
STEPS  
→

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AB  
YIELD 55%

RX(24) RCT F 41838-25-9, AY 555-16-8

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

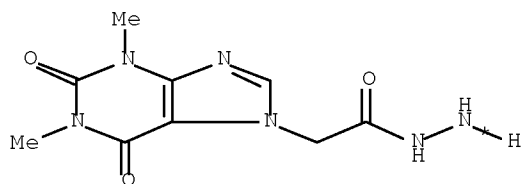
STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

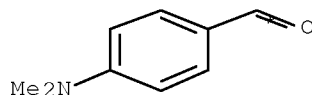
PRO AZ 901781-65-5  
NTE intermediate was isolated

RX(31) RCT AZ 901781-65-5  
RGT Q 7719-09-7 SOCl2  
PRO AB 901781-72-4  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(51) OF 139 COMPOSED OF RX(25), RX(32)  
RX(51) F + BA + J ==> AD

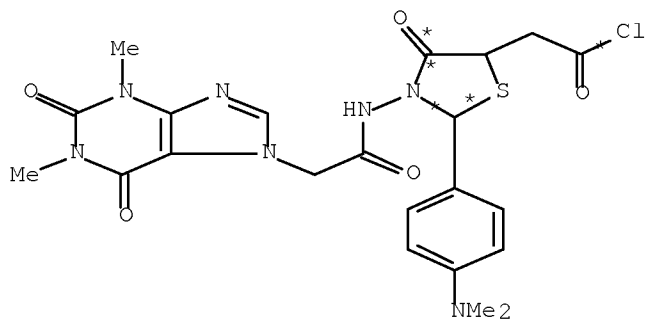
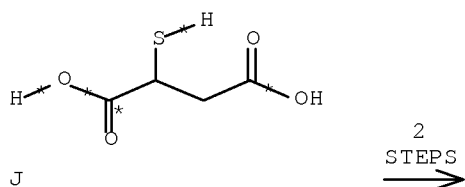


F



BA

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AD  
YIELD 60%

RX(25) RCT F 41838-25-9, BA 100-10-7

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

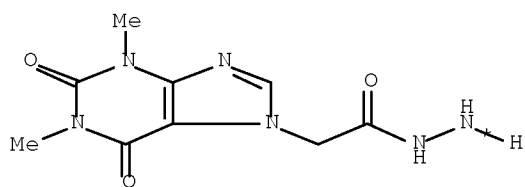
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO BB 901781-66-6  
NTE intermediate was isolated

RX(32) RCT BB 901781-66-6  
RGT Q 7719-09-7 SOCl2  
PRO AD 901781-73-5  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(52) OF 139 COMPOSED OF RX(26), RX(33)  
RX(52) F + BC + J ==> AF

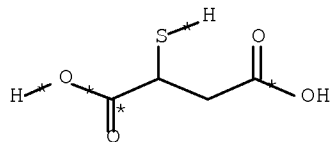
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F

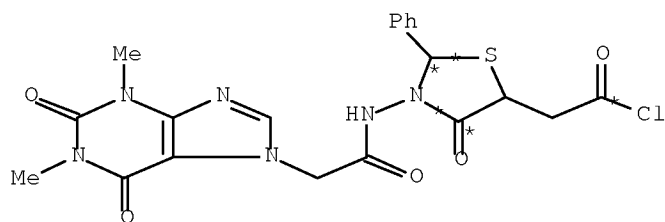


BC



J

2  
STEPS  
→



AF  
YIELD 48%

RX(26) RCT F 41838-25-9, BC 100-52-7

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

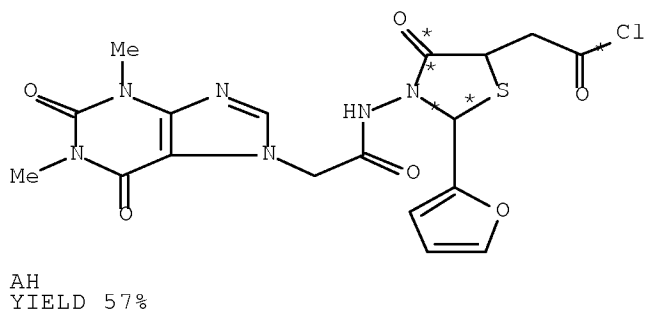
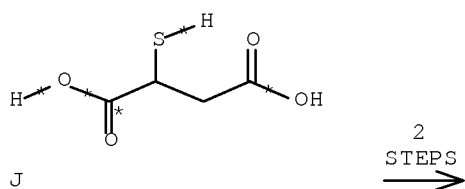
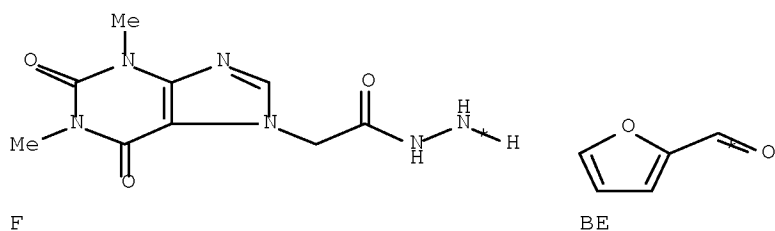
RCT J 70-49-5  
CAT 7646-85-7 ZnCl<sub>2</sub>  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO BD 901781-67-7  
NTE intermediate was isolated

RX(33) RCT BD 901781-67-7  
RGT Q 7719-09-7 SOCl<sub>2</sub>  
PRO AF 901781-74-6  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(53) OF 139 COMPOSED OF RX(27), RX(34)  
RX(53) F + BE + J ==> AH

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RX(27) RCT F 41838-25-9, BE 98-01-1

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl<sub>2</sub>  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO BF 901781-68-8  
NTE intermediate was isolated

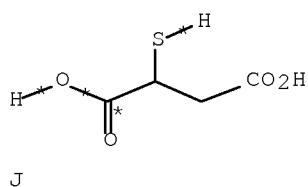
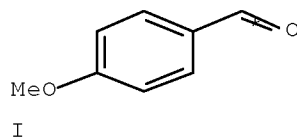
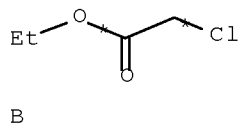
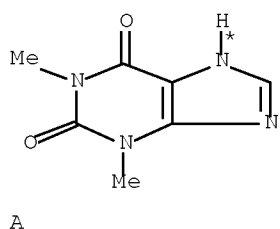
RX(34) RCT BF 901781-68-8



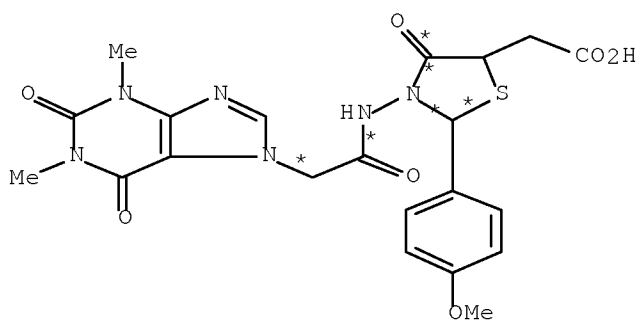
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RGT Q 7719-09-7 SOC12  
PRO AH 901781-75-7  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(68) OF 139 COMPOSED OF RX(1), RX(2), RX(3)  
RX(68) A + B + I + J ==> K



3  
STEPS  
→



YIELD 60%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

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STAGE(2)

RCT B 105-39-5  
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(3) RCT F 41838-25-9, I 123-11-5

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

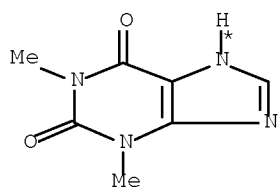
STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

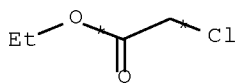
PRO K 901781-44-0  
NTE intermediate was isolated

RX(69) OF 139 COMPOSED OF RX(1), RX(2), RX(21)

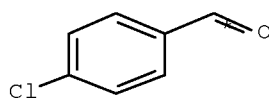
RX(69) A + B + AS + J ==> AT



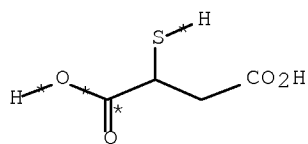
A



B



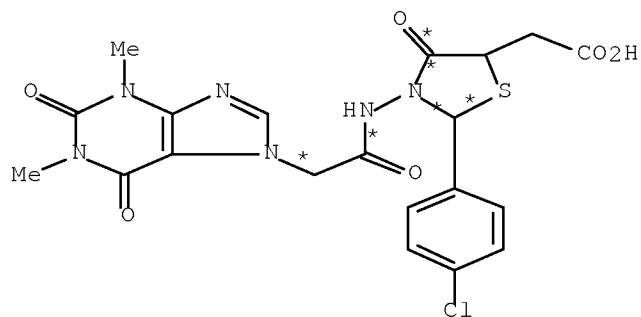
AS



J

3  
STEPS  
→

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AT  
YIELD 59%

RX(1) RCT A 58-55-9  
STAGE(1)  
RGT D 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

STAGE(2)  
RCT B 105-39-5  
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(21) RCT F 41838-25-9, AS 104-88-1

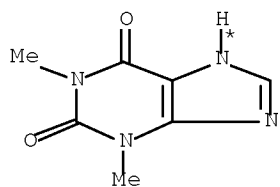
STAGE(1)  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)  
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

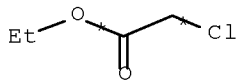
PRO AT 901781-62-2  
NTE intermediate was isolated

RX(70) OF 139 COMPOSED OF RX(1), RX(2), RX(22)  
RX(70) A + B + AU + J ==> AV

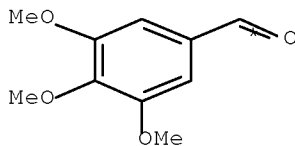
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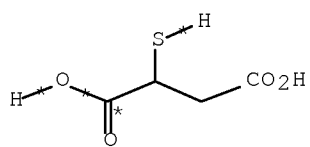
A



B

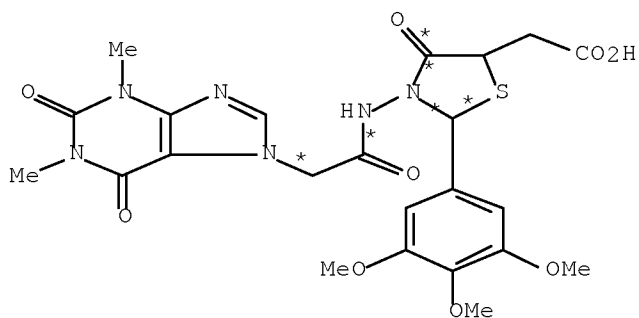


AU



J

3  
STEPS  
→



AV  
YIELD 63%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5

CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1

RGT G 7803-57-8 N2H4-H2O

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PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(22) RCT F 41838-25-9, AU 86-81-7

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

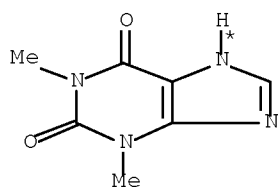
STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

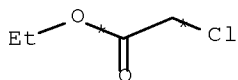
PRO AV 901781-63-3  
NTE intermediate was isolated

RX(71) OF 139 COMPOSED OF RX(1), RX(2), RX(23)

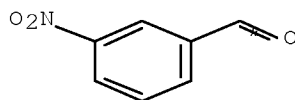
RX(71) A + B + AW + J ==> AX



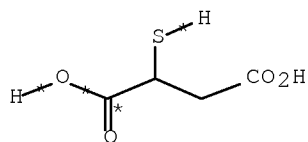
A



B



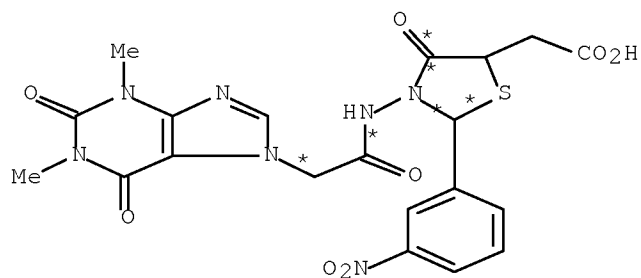
AW



J

3  
STEPS  
→

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AX  
YIELD 67%

RX(1) RCT A 58-55-9

STAGE(1)  
RGT D 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

STAGE(2)  
RCT B 105-39-5  
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(23) RCT F 41838-25-9, AW 99-61-6

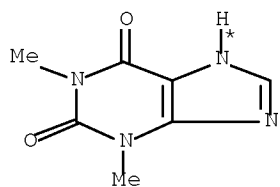
STAGE(1)  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)  
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

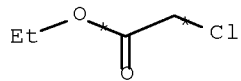
PRO AX 901781-64-4  
NTE intermediate was isolated

RX(72) OF 139 COMPOSED OF RX(1), RX(2), RX(24)  
RX(72) A + B + AY + J ==> AZ

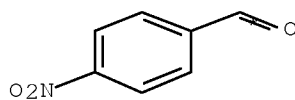
10/595943



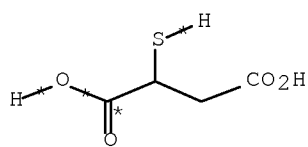
A



B

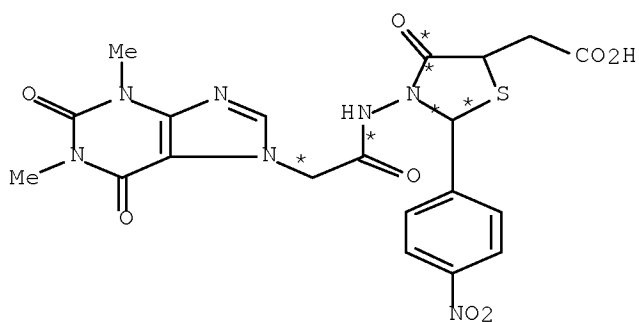


AY



J

3  
STEPS  
→



AZ  
YIELD 61%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5

CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1

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RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(24) RCT F 41838-25-9, AY 555-16-8

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

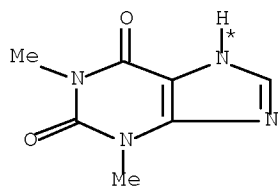
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO AZ 901781-65-5

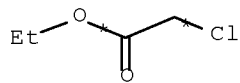
NTE intermediate was isolated

RX(73) OF 139 COMPOSED OF RX(1), RX(2), RX(25)

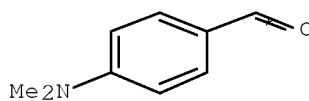
RX(73) A + B + BA + J ==> BB



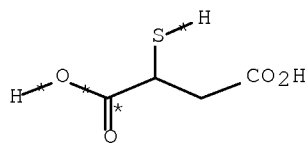
A



B



BA

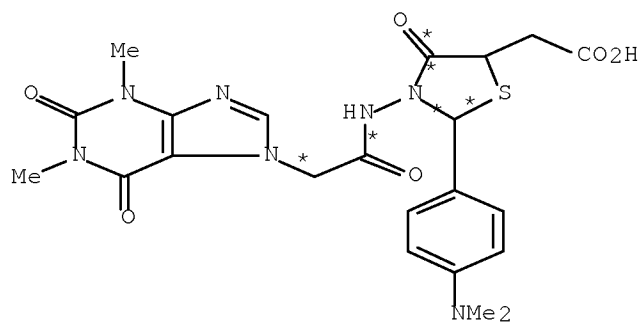


J

3  
STEPS  
→



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BB  
YIELD 57%

RX(1) RCT A 58-55-9  
STAGE(1)  
RGT D 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

STAGE(2)  
RCT B 105-39-5  
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(25) RCT F 41838-25-9, BA 100-10-7

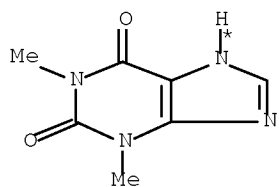
STAGE(1)  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)  
RCT J 70-49-5  
CAT 7646-85-7 ZnCl<sub>2</sub>  
SOL 109-99-9 THF  
CON 10 hours, reflux

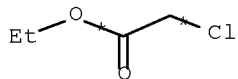
PRO BB 901781-66-6  
NTE intermediate was isolated

RX(74) OF 139 COMPOSED OF RX(1), RX(2), RX(26)  
RX(74) A + B + BC + J ==> ED

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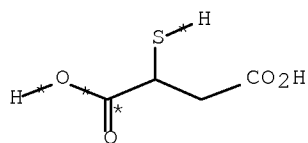
A



B

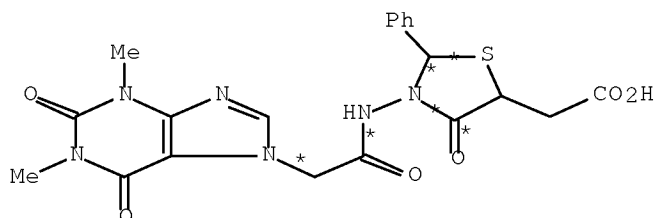


BC



J

3  
STEPS  
→



BD  
YIELD 70%

```

RX(1)      RCT  A 58-55-9

            STAGE(1)
            RGT  D 7646-69-7 NaH
            SOL  68-12-2 DMF
            CON  2 hours, room temperature

            STAGE(2)
            RCT  B 105-39-5
            CON  6 hours, reflux

            PRO  C 7029-96-1

RX(2)      RCT  C 7029-96-1
            RGT  G 7803-57-8 N2H4-H2O
            PRO  F 41838-25-9
            SOL  123-91-1 Dioxane
            CON  6 hours, reflux
  
```

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RX(26) RCT F 41838-25-9, BC 100-52-7

STAGE(1)

CAT 64-19-7 AcOH

SOL 64-17-5 EtOH

CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5

CAT 7646-85-7 ZnCl<sub>2</sub>

SOL 109-99-9 THF

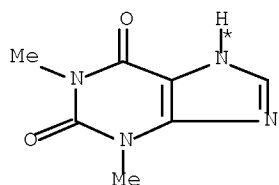
CON 10 hours, reflux

PRO BD 901781-67-7

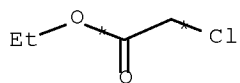
NTE intermediate was isolated

RX(75) OF 139 COMPOSED OF RX(1), RX(2), RX(27)

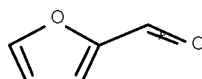
RX(75) A + B + BE + J ==> BF



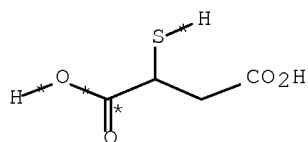
A



B



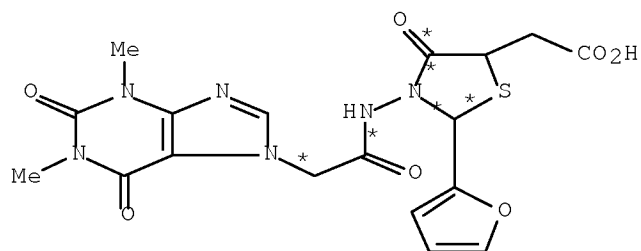
BE



J

3  
STEPS  
→

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BF  
YIELD 69%

RX(1) RCT A 58-55-9  
STAGE(1)  
RGT D 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

STAGE(2)  
RCT B 105-39-5  
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(27) RCT F 41838-25-9, BE 98-01-1

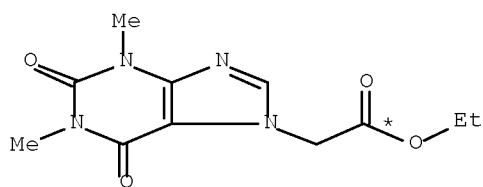
STAGE(1)  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)  
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

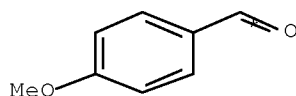
PRO BF 901781-68-8  
NTE intermediate was isolated

RX(76) OF 139 COMPOSED OF RX(2), RX(3), RX(4)  
RX(76) C + I + J ==> F

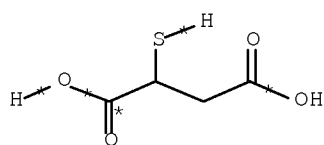
10/595943



C

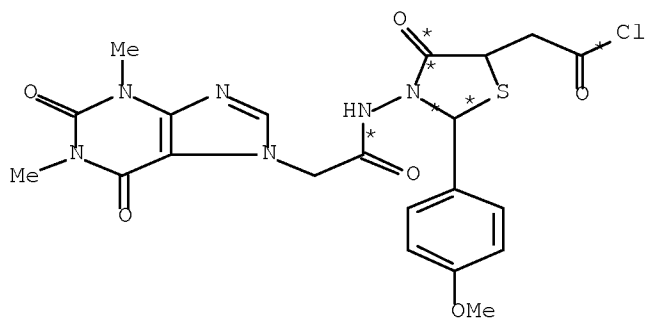


I



J

3  
STEPS  
→



P  
YIELD 43%

RX(2)      RCT   C 7029-96-1  
              RGT   G 7803-57-8 N2H4-H2O  
              PRO   F 41838-25-9  
              SOL   123-91-1 Dioxane  
              CON   6 hours, reflux

RX(3)      RCT   F 41838-25-9, I 123-11-5

STAGE(1)

CAT   64-19-7 AcOH  
 SOL   64-17-5 EtOH  
 CON   5 hours, reflux

STAGE(2)

RCT   J 70-49-5

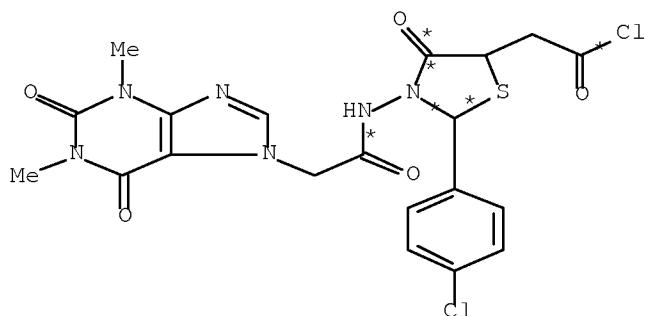
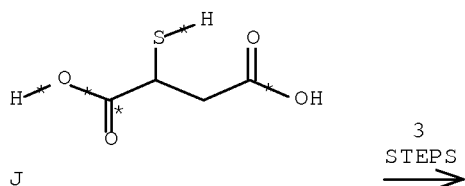
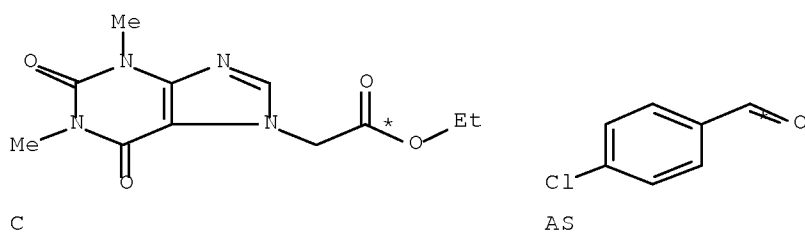
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CAT 7646-85-7 ZnCl<sub>2</sub>  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO K 901781-44-0  
NTE intermediate was isolated

RX(4) RCT K 901781-44-0  
RGT Q 7719-09-7 SOCl<sub>2</sub>  
PRO P 901781-45-1  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(77) OF 139 COMPOSED OF RX(2), RX(21), RX(28)  
RX(77) C + AS + J ==> V



V  
YIELD 52%

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RX(2)        RCT   C 7029-96-1  
              RGT   G 7803-57-8 N2H4-H2O  
              PRO   F 41838-25-9  
              SOL   123-91-1 Dioxane  
              CON   6 hours, reflux

RX(21)      RCT   F 41838-25-9, AS 104-88-1

              STAGE(1)

                 CAT   64-19-7 AcOH  
                 SOL   64-17-5 EtOH  
                 CON   5 hours, reflux

              STAGE(2)

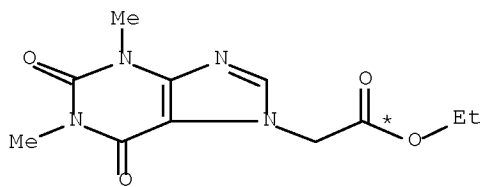
                 RCT   J 70-49-5  
                 CAT   7646-85-7 ZnCl2  
                 SOL   109-99-9 THF  
                 CON   10 hours, reflux

              PRO   AT 901781-62-2  
              NTE   intermediate was isolated

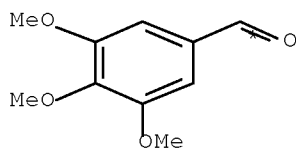
RX(28)      RCT   AT 901781-62-2  
              RGT   Q 7719-09-7 SOCl2  
              PRO   V 901781-69-9  
              SOL   108-88-3 PhMe  
              CON   30 minutes, reflux

RX(78) OF 139 COMPOSED OF RX(2), RX(22), RX(29)

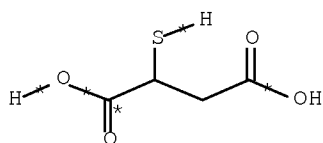
RX(78)      C   +   AU   +   J   ==>   X



C



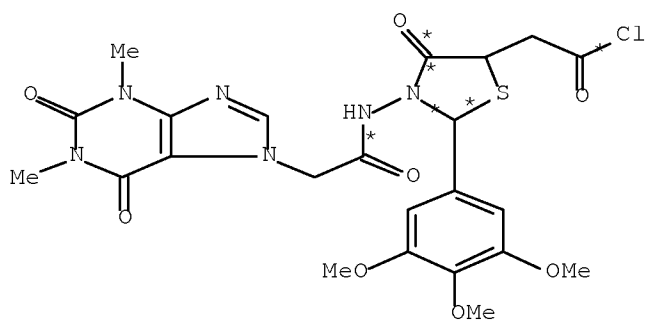
AU



J

3  
STEPS  
→

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X  
YIELD 47%

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(22) RCT F 41838-25-9, AU 86-81-7

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO AV 901781-63-3  
NTE intermediate was isolated

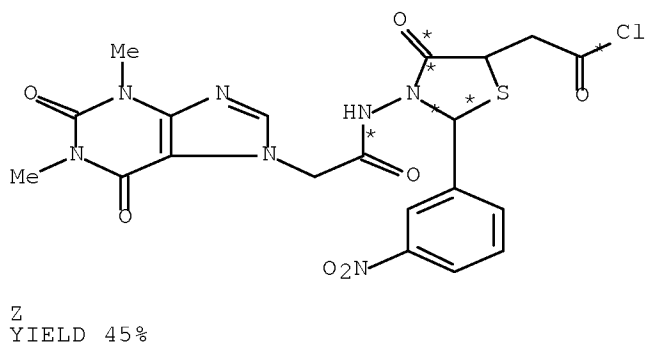
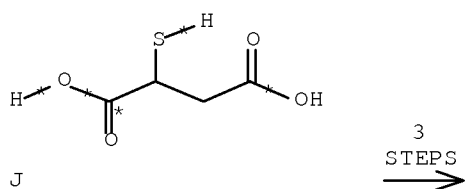
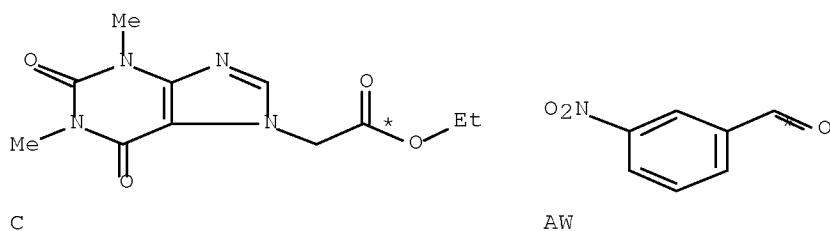
RX(29) RCT AV 901781-63-3  
RGT Q 7719-09-7 SOCl2  
PRO X 901781-70-2  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(79) OF 139 COMPOSED OF RX(2), RX(23), RX(30)

RX(79) C + AW + J ==> Z



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RX(2)        RCT   C 7029-96-1  
              RGT   G ~~7803-57-8~~ N2H4-H2O  
              PRO   F 41838-25-9  
              SOL   123-91-1 Dioxane  
              CON   6 hours, reflux

RX(23) RCT F 41838-25-9, AW 99-61-6

```
STAGE(1)
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux
```

```
STAGE(2)
      RCT  J 70--49--5
      CAT  7646--85--7 ZnCl2
```

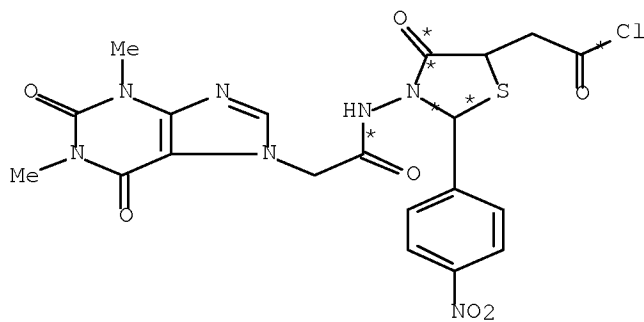
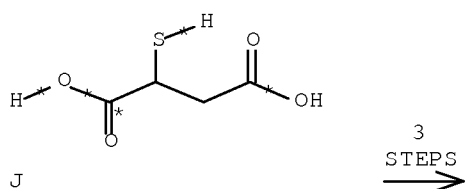
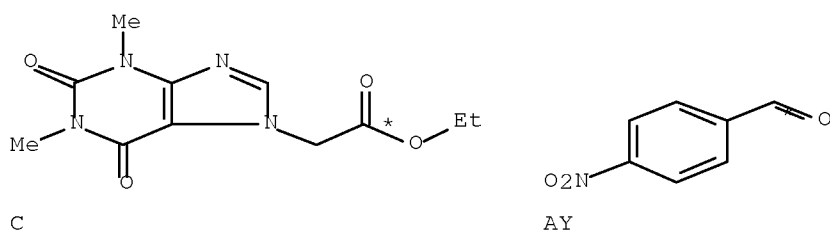
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SOL 109-99-9 THF  
CON 10 hours, reflux

PRO AX 901781-64-4  
NTE intermediate was isolated

RX(30) RCT AX 901781-64-4  
RGT Q 7719-09-7 SOCl<sub>2</sub>  
PRO Z 901781-71-3  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(80) OF 139 COMPOSED OF RX(2), RX(24), RX(31)  
RX(80) C + AY + J ==> AE



AE  
YIELD 55%

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RX(2)        RCT   C 7029-96-1  
              RGT   G 7803-57-8 N2H4-H2O  
              PRO   F 41838-25-9  
              SOL   123-91-1 Dioxane  
              CON   6 hours, reflux

RX(24)       RCT   F 41838-25-9, AY 555-16-8

STAGE(1)

CAT   64-19-7 AcOH  
SOL   64-17-5 EtOH  
CON   5 hours, reflux

STAGE(2)

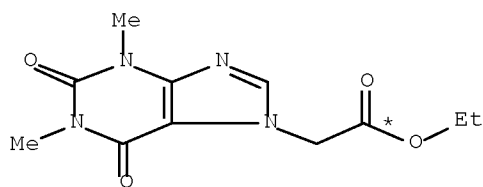
RCT   J 70-49-5  
CAT   7646-85-7 ZnCl2  
SOL   109-99-9 THF  
CON   10 hours, reflux

PRO   AZ 901781-65-5  
NTE   intermediate was isolated

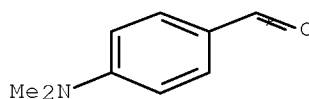
RX(31)       RCT   AZ 901781-65-5  
              RGT   Q 7719-09-7 SOCl2  
              PRO   AB 901781-72-4  
              SOL   108-88-3 PhMe  
              CON   30 minutes, reflux

RX(81) OF 139 COMPOSED OF RX(2), RX(25), RX(32)

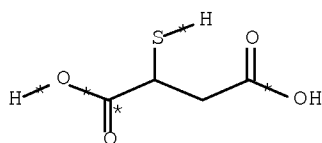
RX(81)       C   +   BA   +   J   ==>   AD



C



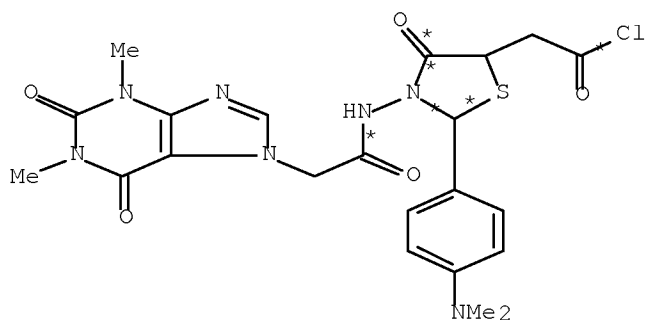
BA



J

3  
STEPS  
→

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AD  
YIELD 60%

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(25) RCT F 41838-25-9, BA 100-10-7

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

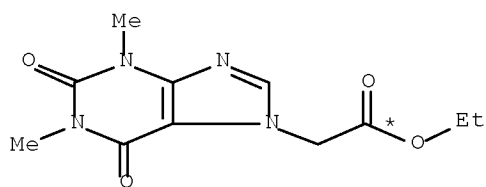
PRO BB 901781-66-6  
NTE intermediate was isolated

RX(32) RCT BB 901781-66-6  
RGT Q 7719-09-7 SOCl2  
PRO AD 901781-73-5  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(82) OF 139 COMPOSED OF RX(2), RX(26), RX(33)

RX(82) C + BC + J ==> AF

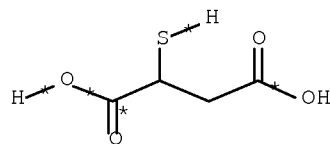
10/595943



C

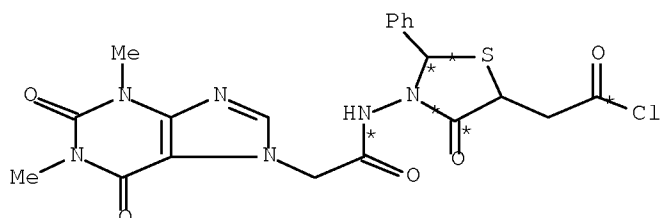


BC



J

3  
STEPS  
→



AF  
YIELD 48%

```

RX(2)      RCT  C 7029-96-1
           RGT  G 7803-57-8 N2H4-H2O
           PRO  F 41838-25-9
           SOL  123-91-1 Dioxane
           CON  6 hours, reflux

RX(26)     RCT  F 41838-25-9, BC 100-52-7

           STAGE(1)
             CAT  64-19-7 AcOH
             SOL  64-17-5 EtOH
             CON  5 hours, reflux

           STAGE(2)
             RCT  J 70-49-5
             CAT  7646-85-7 ZnCl2
             SOL  109-99-9 THF
             CON  10 hours, reflux

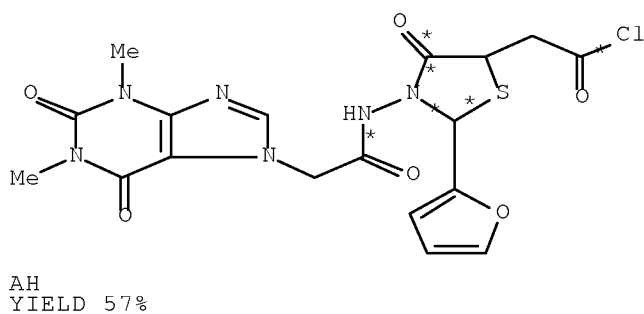
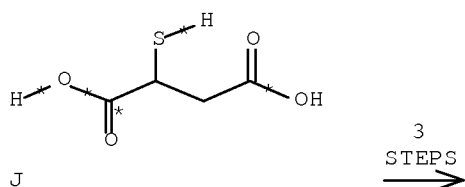
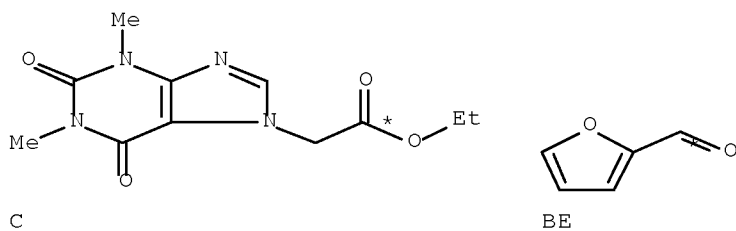
           PRO  BD 901781-67-7
           NTE  intermediate was isolated

RX(33)     RCT  BD 901781-67-7
           RGT  Q 7719-09-7 SOC12
  
```

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PRO AF 901781-74-6  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(83) OF 139 COMPOSED OF RX(2), RX(27), RX(34)  
RX(83) C + BE + J ==> AH



RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(27) RCT F 41838-25-9, BE 98-01-1

STAGE(1)

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CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

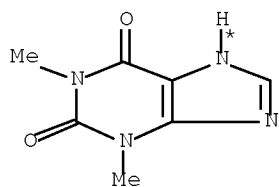
RCT J 70-49-5  
CAT 7646-85-7 ZnCl<sub>2</sub>  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO BF 901781-68-8  
NTE intermediate was isolated

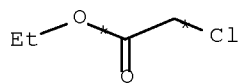
RX(34) RCT BF 901781-68-8  
RGT Q 7719-09-7 SOCl<sub>2</sub>  
PRO AH 901781-75-7  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(84) OF 139 COMPOSED OF RX(1), RX(2), RX(3), RX(4)

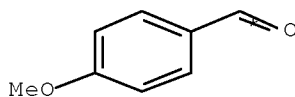
RX(84) A + B + I + J ==> P



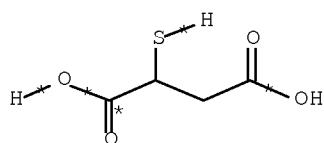
A



B



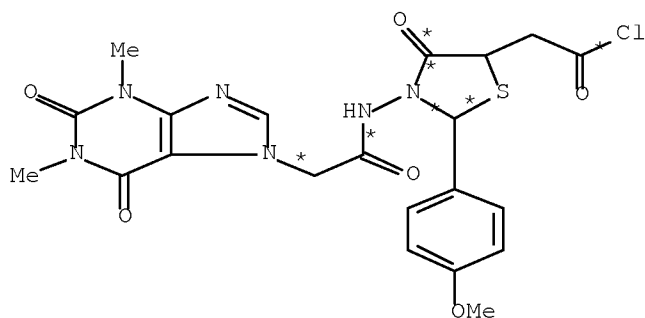
I



J

4  
STEPS  
→

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P  
YIELD 43%

```

RX(1)      RCT   A 58-55-9

              STAGE(1)
                RGT   D 7646-69-7 NaH
                SOL   68-12-2 DMF
                CON   2 hours, room temperature

```

```

STAGE(2)
      RCT  B 105-39-5
      CON  6 hours, reflux

```

PRO C 7029-96-1

RX (2)            RCT   C 7029-96-1  
                  RGT   G ~~7803-57-8~~ N2H4-H2O  
                  PRO   F 41838-25-9  
                  SOL   123-91-1 Dioxane  
                  CON   6 hours, reflux

RX(3) RCT F 41838-25-9, I 123-11-5

STAGE (1)  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE (2)  
 RCT J 70-49-5  
 CAT 7646-85-7 ZnCl2  
 SOL 109-99-9 THF  
 CON 10 hours, reflux

PRO K 901781-44-0  
NTE intermediate was isolated

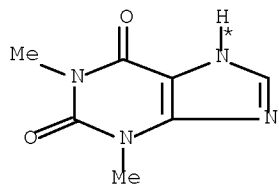
RX (4)	RCT	K 901781-44-0
	RGT	Q 7719-09-7 SOC12
	PRO	P 901781-45-1
	SOL	108-88-3 PhMe
	CON	30 minutes, reflux



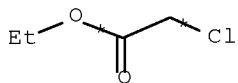
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RX(85) OF 139 COMPOSED OF RX(1), RX(2), RX(21), RX(28)

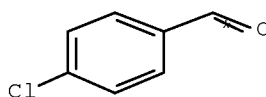
RX(85) A + B + AS + J ==> V



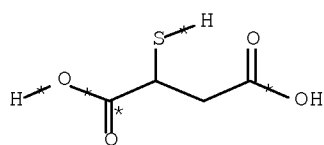
A



B

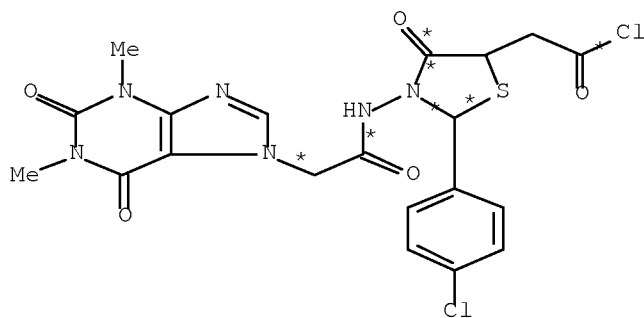


AS



J

4  
STEPS  
→



V  
YIELD 52%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5

CON 6 hours, reflux

PRO C 7029-96-1

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RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(21) RCT F 41838-25-9, AS 104-88-1

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

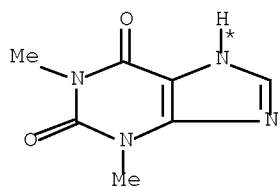
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO AT 901781-62-2  
NTE intermediate was isolated

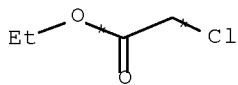
RX(28) RCT AT 901781-62-2  
RGT Q 7719-09-7 SOCl2  
PRO V 901781-69-9  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(86) OF 139 COMPOSED OF RX(1), RX(2), RX(22), RX(29)

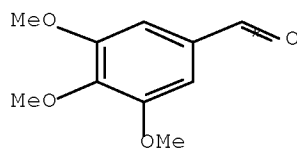
RX(86) A + B + AU + J ==> X



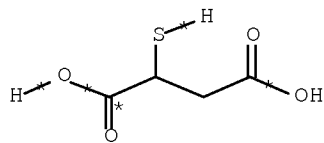
A



B



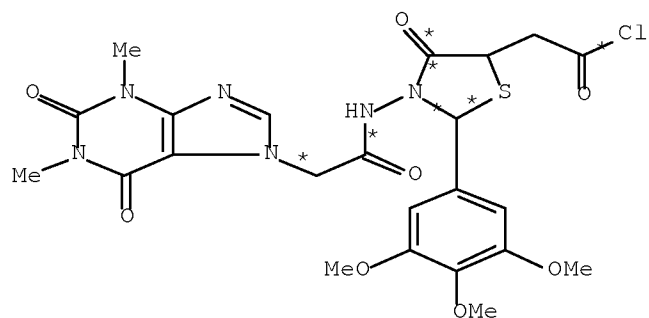
AU



J

4  
STEPS  
→

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X  
YIELD 47%

RX(1) RCT A 58-55-9  
STAGE(1)  
RGT D 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

STAGE(2)  
RCT B 105-39-5  
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(22) RCT F 41838-25-9, AU 86-81-7

STAGE(1)  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)  
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

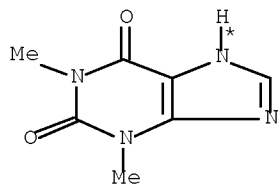
PRO AV 901781-63-3  
NTE intermediate was isolated

RX(29) RCT AV 901781-63-3  
RGT Q 7719-09-7 SOCl2  
PRO X 901781-70-2  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

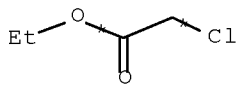
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RX(87) OF 139 COMPOSED OF RX(1), RX(2), RX(23), RX(30)

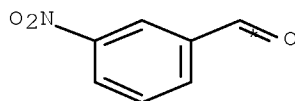
RX(87) A + B + AW + J ==> Z



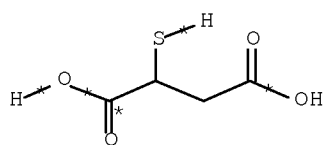
A



B

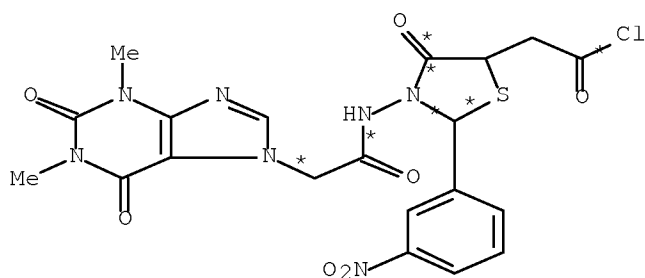


AW



J

4  
STEPS  
➔



Z  
YIELD 45%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5

CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1

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RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(23) RCT F 41838-25-9, AW 99-61-6

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

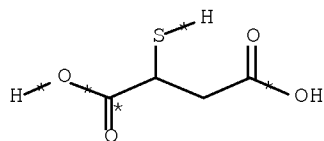
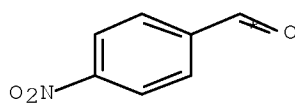
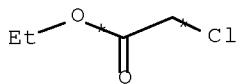
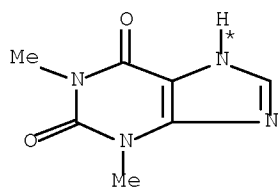
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO AX 901781-64-4  
NTE intermediate was isolated

RX(30) RCT AX 901781-64-4  
RGT Q 7719-09-7 SOCl2  
PRO Z 901781-71-3  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

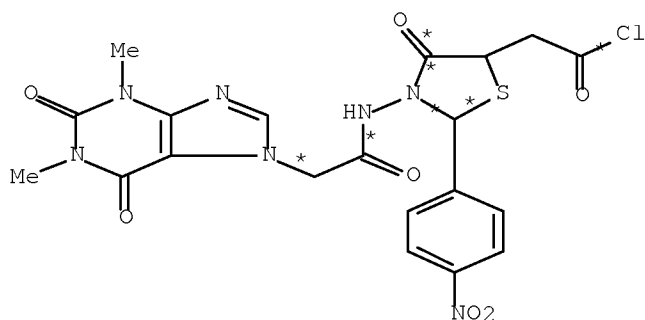
RX(88) OF 139 COMPOSED OF RX(1), RX(2), RX(24), RX(31)

RX(88) A + B + AY + J ==> AB



4  
STEPS  
→

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AB  
YIELD 55%

RX(1) RCT A 58-55-9

STAGE(1)  
RGT D 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

STAGE(2)  
RCT B 105-39-5  
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(24) RCT F 41838-25-9, AY 555-16-8

STAGE(1)  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)  
RCT J 70-49-5  
CAT 7646-85-7 ZnCl<sub>2</sub>  
SOL 109-99-9 THF  
CON 10 hours, reflux

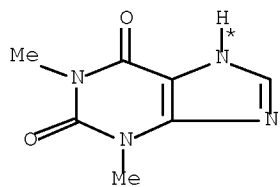
PRO AZ 901781-65-5  
NTE intermediate was isolated

RX(31) RCT AZ 901781-65-5  
RGT Q 7719-09-7 SOCl<sub>2</sub>  
PRO AB 901781-72-4  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

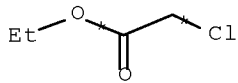
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RX(89) OF 139 COMPOSED OF RX(1), RX(2), RX(25), RX(32)

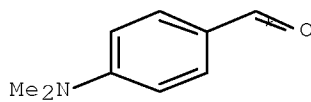
RX(89) A + B + BA + J ==> AD



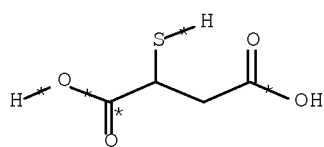
A



B

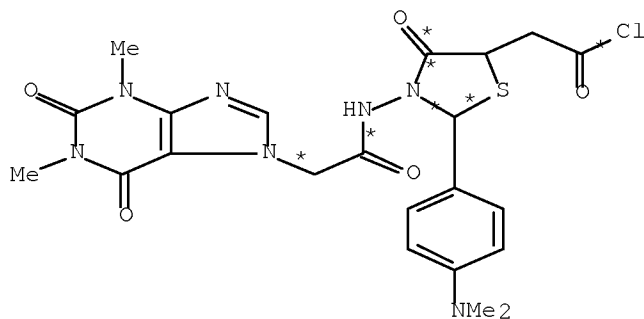


BA



J

4  
STEPS  
→



AD  
YIELD 60%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5

CON 6 hours, reflux

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PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
 RGT G ~~7803-57-8~~ N2H4-H2O  
 PRO F 41838-25-9  
 SOL 123-91-1 Dioxane  
 CON 6 hours, reflux

RX(25) RCT F 41838-25-9, BA 100-10-7

STAGE(1)  
 CAT 64-19-7 AcOH  
 SOL 64-17-5 EtOH  
 CON 5 hours, reflux

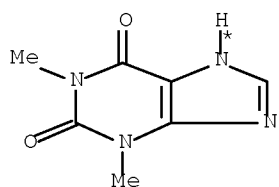
STAGE(2)  
 RCT J ~~70-49-5~~  
 CAT ~~7646-85-7~~ ZnCl2  
 SOL 109-99-9 THF  
 CON 10 hours, reflux

PRO BB 901781-66-6  
 NTE intermediate was isolated

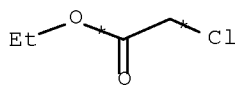
RX(32) RCT BB 901781-66-6  
 RGT Q 7719-09-7 SOCl2  
 PRO AD ~~901781-73-5~~  
 SOL 108-88-3 PhMe  
 CON 30 minutes, reflux

RX(90) OF 139 COMPOSED OF RX(1), RX(2), RX(26), RX(33)

RX(90) A + B + BC + J ==> AF



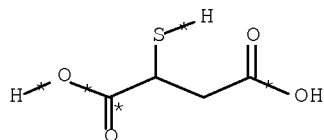
A



B



BC

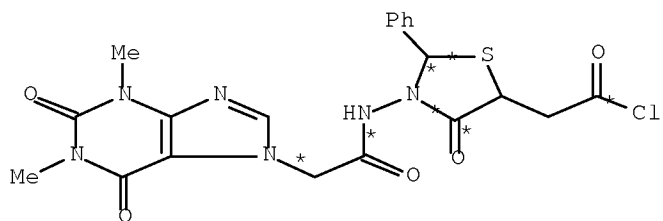


J

4  
 STEPS  
 →



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AF  
YIELD 48%

RX(1) RCT A 58-55-9

STAGE(1)  
RGT D 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

STAGE(2)  
RCT B 105-39-5  
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(26) RCT F 41838-25-9, BC 100-52-7

STAGE(1)  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

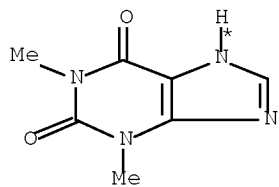
STAGE(2)  
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO BD 901781-67-7  
NTE intermediate was isolated

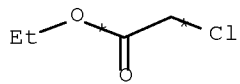
RX(33) RCT BD 901781-67-7  
RGT Q 7719-09-7 SOCl2  
PRO AF 901781-74-6  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(91) OF 139 COMPOSED OF RX(1), RX(2), RX(27), RX(34)  
RX(91) A + B + BE + J ==> AH

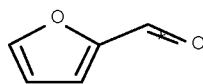
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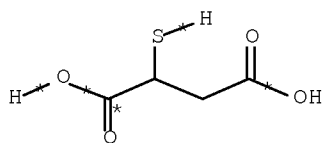
A



B

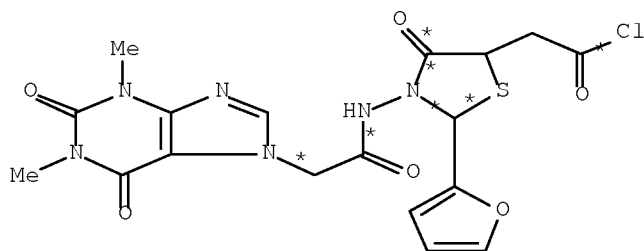


BE



J

4  
STEPS  
→



AH  
YIELD 57%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5

CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9

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SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(27) RCT F 41838-25-9, BE 98-01-1

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

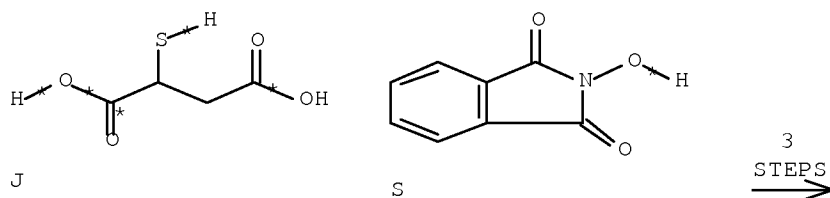
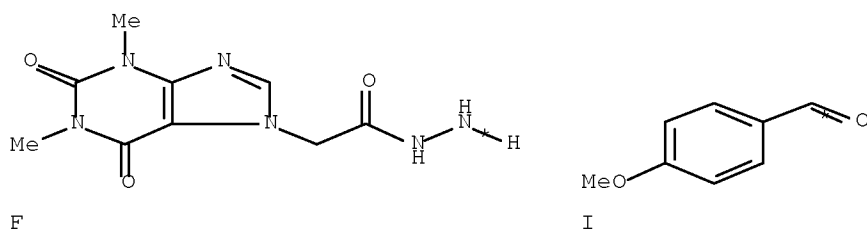
RCT J 76-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO BF 901781-68-8  
NTE intermediate was isolated

RX(34) RCT BF 901781-68-8  
RGT Q 7719-09-7 SOCl2  
PRO AH 901781-75-7  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(92) OF 139 COMPOSED OF RX(3), RX(4), RX(5)

RX(92) F + I + J + S ==> T



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(3) RCT F 41838-25-9, I 123-11-5

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STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

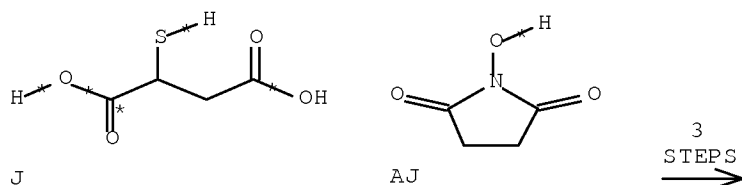
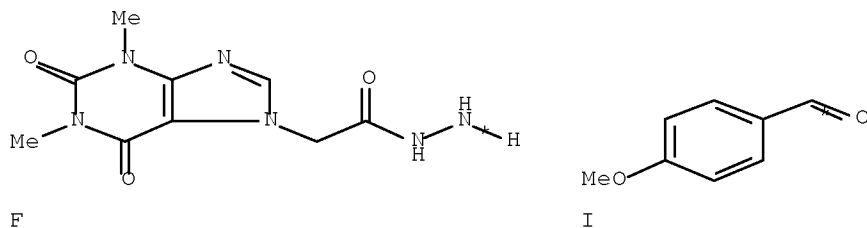
PRO K 901781-44-0  
NTE intermediate was isolated

RX(4) RCT K 901781-44-0  
RGT Q 7719-09-7 SOCl2  
PRO P 901781-45-1  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

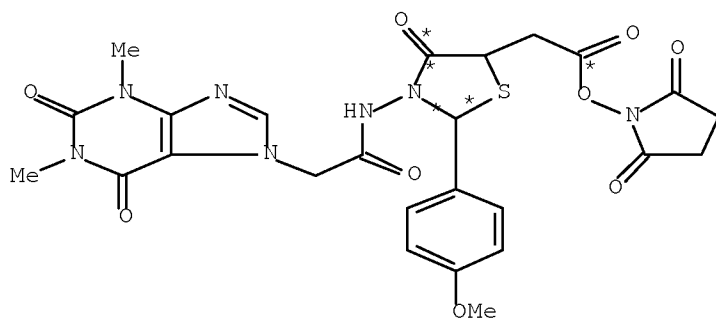
RX(5) RCT P 901781-45-1, S 524-38-9  
RGT U 121-44-8 Et3N  
PRO T 901781-46-2  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

RX(93) OF 139 COMPOSED OF RX(3), RX(4), RX(13)

RX(93) F + I + J + AJ ==> AK



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AK  
YIELD 70%

RX(3) RCT F 41838-25-9, I 123-11-5

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

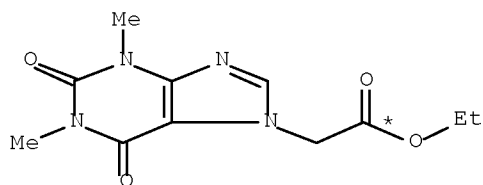
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO K 901781-44-0  
NTE intermediate was isolated

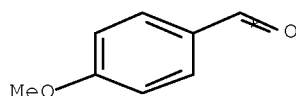
RX(4) RCT K 901781-44-0  
RGT Q 7719-09-7 SOCl2  
PRO P 901781-45-1  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(13) RCT P 901781-45-1, AJ 6066-82-6  
RGT U 121-44-8 Et3N  
PRO AK 901781-54-2  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

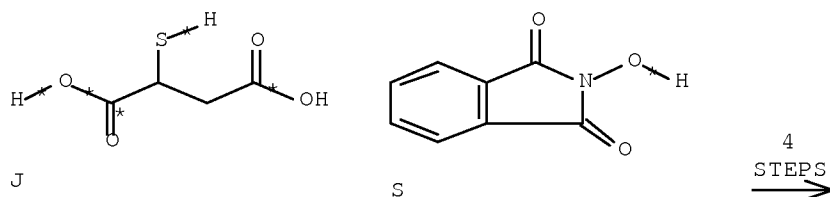
RX(94) OF 139 COMPOSED OF RX(2), RX(3), RX(4), RX(5)  
RX(94) C + I + J + S ==> T



C



I



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

```

RX(2)      RCT  C 7029-96-1
           RGT  G 7803-57-8 N2H4-H2O
           PRO  F 41838-25-9
           SOL  123-91-1 Dioxane
           CON  6 hours, reflux

RX(3)      RCT  F 41838-25-9, I 123-11-5

           STAGE(1)
             CAT  64-19-7 AcOH
             SOL  64-17-5 EtOH
             CON  5 hours, reflux

           STAGE(2)
             RCT  J 70-49-5
             CAT  7646-85-7 ZnCl2
             SOL  109-99-9 THF
             CON  10 hours, reflux

           PRO  K 901781-44-0
           NTE  intermediate was isolated

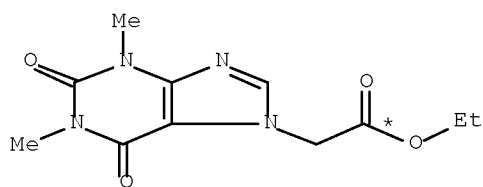
RX(4)      RCT  K 901781-44-0
           RGT  Q 7719-09-7 SOCl2
           PRO  P 901781-45-1
           SOL  108-88-3 PhMe
           CON  30 minutes, reflux

RX(5)      RCT  P 901781-45-1, S 524-38-9
           RGT  U 121-44-8 Et3N
           PRO  T 901781-46-2
           SOL  68-12-2 DMF
           CON  6 hours, room temperature
  
```

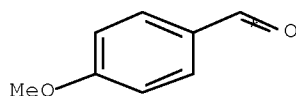
```

RX(95) OF 139 COMPOSED OF RX(2), RX(3), RX(4), RX(13)
RX(95)    C  +  I  +  J  +  AJ  ==>  AK
  
```

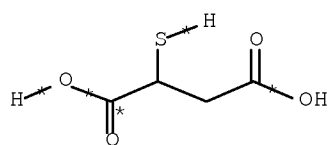
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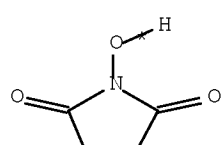
C



I

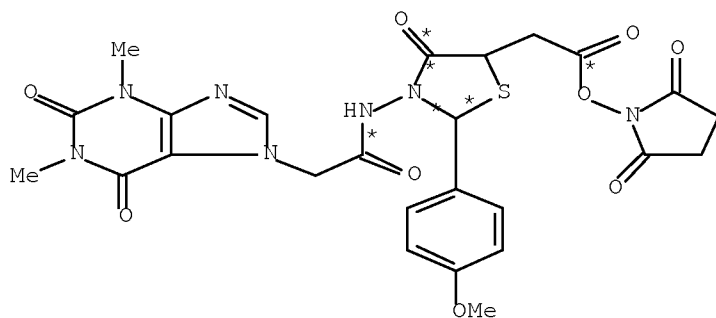


J



AJ

4  
STEPS  
→



AK  
YIELD 70%

RX(2)      RCT   C 7029-96-1  
              RGT   G 7803-57-8 N2H4-H2O  
              PRO   F 41838-25-9  
              SOL   123-91-1 Dioxane  
              CON   6 hours, reflux

RX(3)      RCT   F 41838-25-9, I 123-11-5

STAGE(1)

CAT   64-19-7 AcOH  
 SOL   64-17-5 EtOH  
 CON   5 hours, reflux

STAGE(2)

RCT   J 70-49-5

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CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

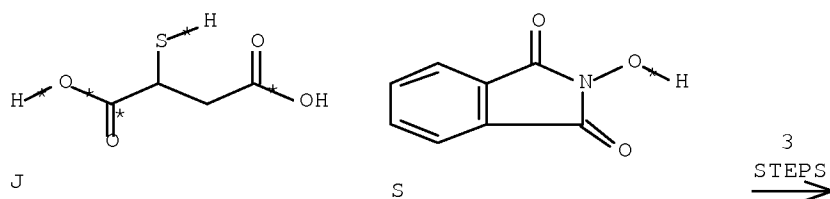
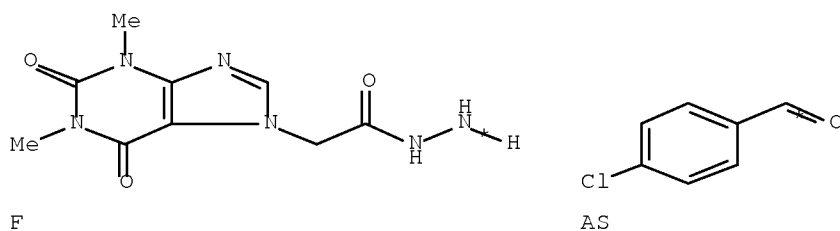
PRO K 901781-44-0  
NTE intermediate was isolated

RX(4) RCT K 901781-44-0  
RGT Q 7719-09-7 SOCl2  
PRO P 901781-45-1  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(13) RCT P 901781-45-1, AJ 6066-82-6  
RGT U 121-44-8 Et3N  
PRO AK 901781-54-2  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

RX(96) OF 139 COMPOSED OF RX(21), RX(28), RX(6)

RX(96) F + AS + J + S ==> W



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(21) RCT F 41838-25-9, AS 104-88-1

STAGE(1)  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux



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STAGE(2)

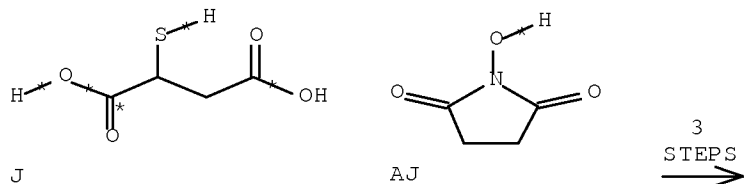
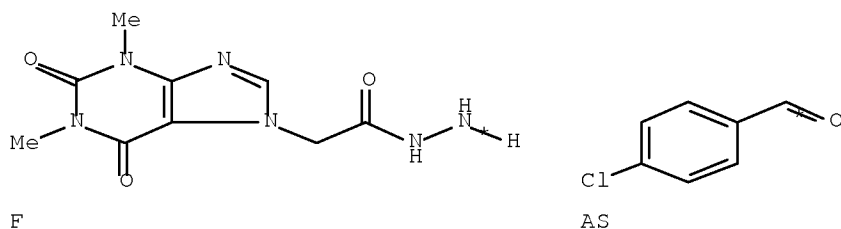
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO AT 901781-62-2  
NTE intermediate was isolated

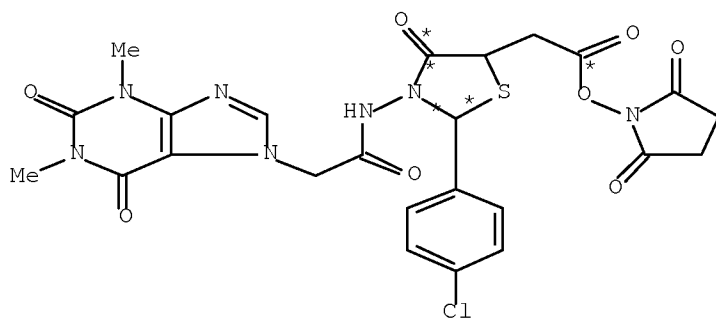
RX(28) RCT AT 901781-62-2  
RGT Q 7719-09-7 SOCl2  
PRO V 901781-69-9  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(6) RCT V 901781-69-9, S 524-38-9  
RGT U 121-44-8 Et3N  
PRO W 901781-47-3  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

RX(97) OF 139 COMPOSED OF RX(21), RX(28), RX(14)  
RX(97) F + AS + J + AJ ==> AL



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AL  
YIELD 62%

RX(21) RCT F 41838-25-9, AS 104-88-1

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

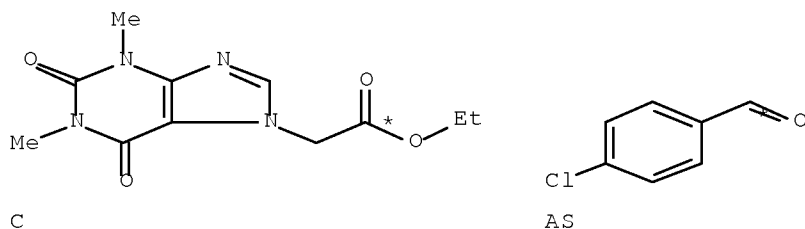
PRO AT 901781-62-2  
NTE intermediate was isolated

RX(28) RCT AT 901781-62-2  
RGT Q 7719-09-7 SOCl2  
PRO V 901781-69-9  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(14) RCT V 901781-69-9, AJ 6066-82-6  
RGT U 121-44-8 Et3N  
PRO AL 901781-55-3  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

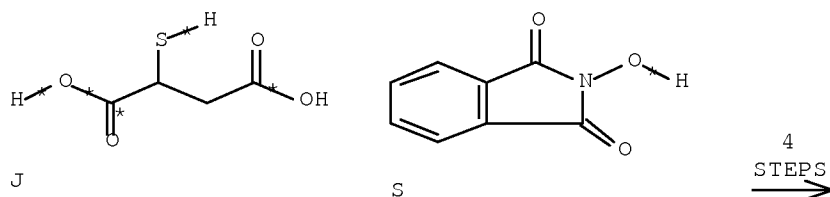
RX(98) OF 139 COMPOSED OF RX(2), RX(21), RX(28), RX(6)

RX(98) C + AS + J + S ==> W



C

AS



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT C 7029-96-1  
 RGT G 7803-57-8 N2H4-H2O  
 PRO F 41838-25-9  
 SOL 123-91-1 Dioxane  
 CON 6 hours, reflux

RX(21) RCT F 41838-25-9, AS 104-88-1

STAGE(1)

CAT 64-19-7 AcOH  
 SOL 64-17-5 EtOH  
 CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5  
 CAT 7646-85-7 ZnCl2  
 SOL 109-99-9 THF  
 CON 10 hours, reflux

PRO AT 901781-62-2  
 NTE intermediate was isolated

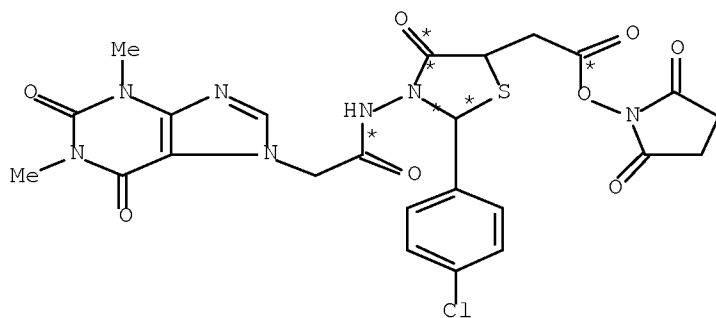
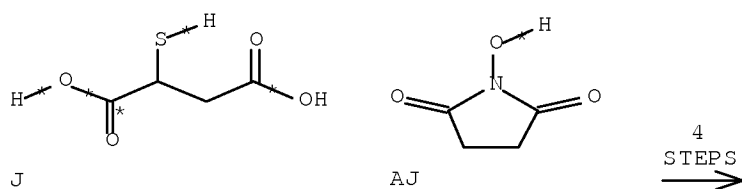
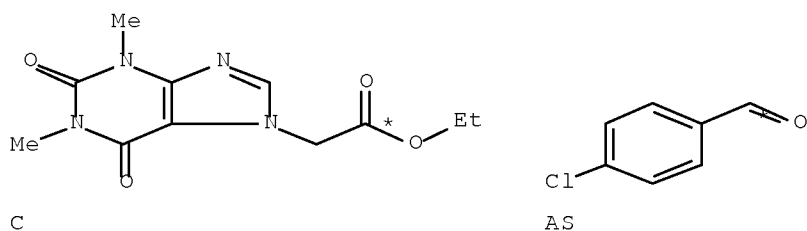
RX(28) RCT AT 901781-62-2  
 RGT Q 7719-09-7 SOCl2  
 PRO V 901781-69-9  
 SOL 108-88-3 PhMe  
 CON 30 minutes, reflux

RX(6) RCT V 901781-69-9, S 524-38-9  
 RGT U 121-44-8 Et3N  
 PRO W 901781-47-3  
 SOL 68-12-2 DMF  
 CON 6 hours, room temperature

RX(99) OF 139 COMPOSED OF RX(2), RX(21), RX(28), RX(14)

RX(99) C + AS + J + AJ ==> AL

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YIELD 62%

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(21) RCT F 41838-25-9, AS 104-88-1

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5

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CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

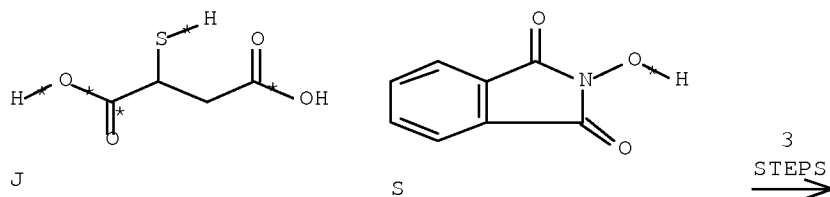
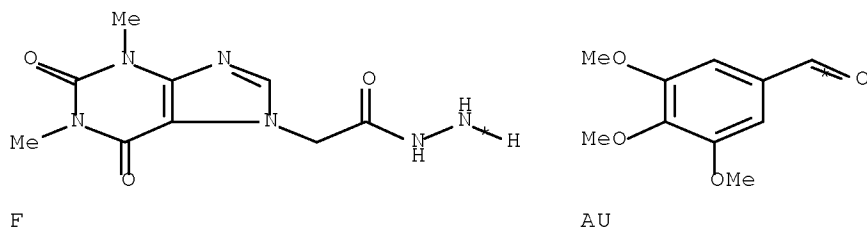
PRO AT 901781-62-2  
NTE intermediate was isolated

RX(28) RCT AT 901781-62-2  
RGT Q 7719-09-7 SOCl2  
PRO V 901781-69-9  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(14) RCT V 901781-69-9, AJ 6066-82-6  
RGT U 121-44-8 Et3N  
PRO AL 901781-55-3  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

RX(100) OF 139 COMPOSED OF RX(22), RX(29), RX(7)

RX(100) F + AU + J + S ==> Y



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(22) RCT F 41838-25-9, AU 86-81-7

STAGE(1)  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

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STAGE(2)

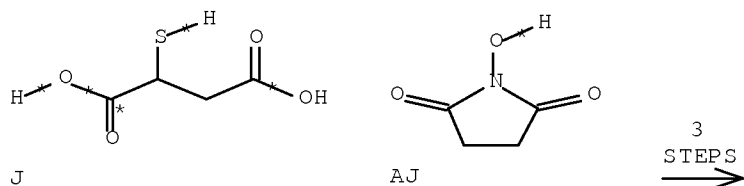
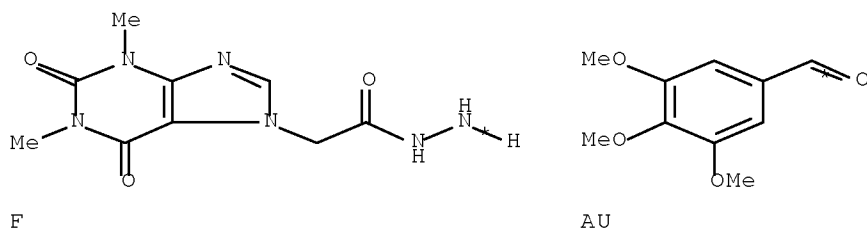
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO AV 901781-63-3  
NTE intermediate was isolated

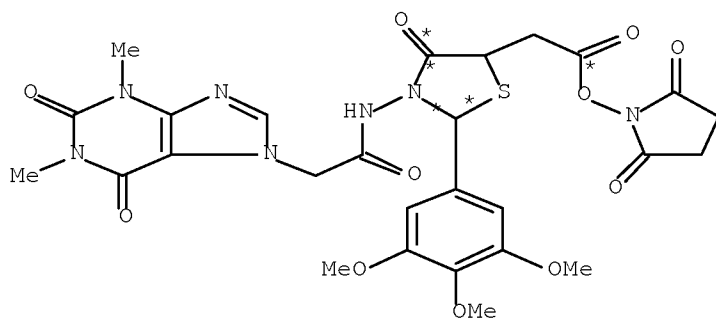
RX(29) RCT AV 901781-63-3  
RGT Q 7719-09-7 SOCl2  
PRO X 901781-70-2  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(7) RCT X 901781-70-2, S 524-38-9  
RGT U 121-44-8 Et3N  
PRO Y 901781-48-4  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

RX(101) OF 139 COMPOSED OF RX(22), RX(29), RX(15)  
RX(101) F + AU + J + AJ ==> AM



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AM  
YIELD 64%

RX(22) RCT F 41838-25-9, AU 86-81-7

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

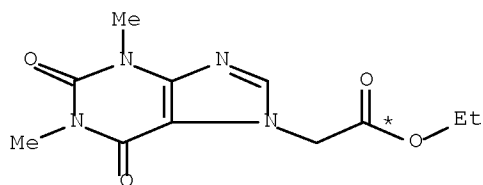
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO AV 901781-63-3  
NTE intermediate was isolated

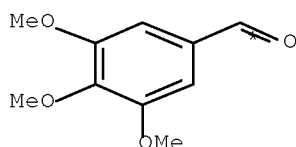
RX(29) RCT AV 901781-63-3  
RGT Q 7719-09-7 SOCl2  
PRO X 901781-70-2  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(15) RCT X 901781-70-2, AJ 6066-82-6  
RGT U 121-44-8 Et3N  
PRO AM 901781-56-4  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

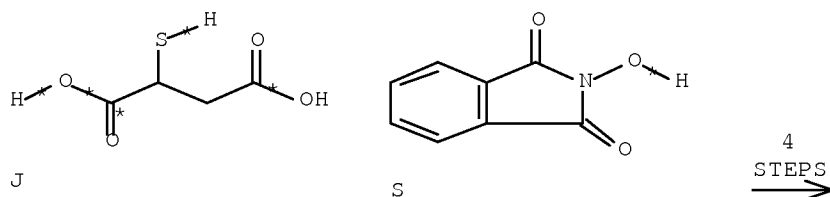
RX(102) OF 139 COMPOSED OF RX(2), RX(22), RX(29), RX(7)  
RX(102) C + AU + J + S ==> Y



C



AU



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

```

RX(2)      RCT  C 7029-96-1
           RGT  G 7803-57-8 N2H4-H2O
           PRO  F 41838-25-9
           SOL  123-91-1 Dioxane
           CON  6 hours, reflux

RX(22)     RCT  F 41838-25-9, AU 86-81-7

           STAGE(1)
             CAT  64-19-7 AcOH
             SOL  64-17-5 EtOH
             CON  5 hours, reflux

           STAGE(2)
             RCT  J 70-49-5
             CAT  7646-85-7 ZnCl2
             SOL  109-99-9 THF
             CON  10 hours, reflux

           PRO  AV 901781-63-3
           NTE  intermediate was isolated

RX(29)     RCT  AV 901781-63-3
           RGT  Q 7719-09-7 SOCl2
           PRO  X 901781-70-2
           SOL  108-88-3 PhMe
           CON  30 minutes, reflux

RX(7)      RCT  X 901781-70-2, S 524-38-9
           RGT  U 121-44-8 Et3N
           PRO  Y 901781-48-4
           SOL  68-12-2 DMF
           CON  6 hours, room temperature

```

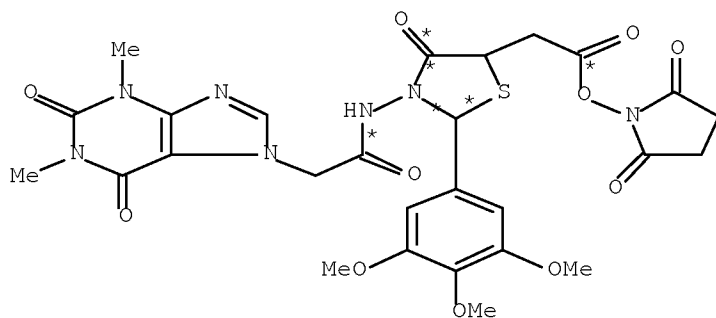
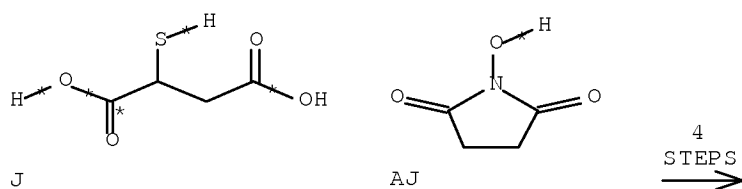
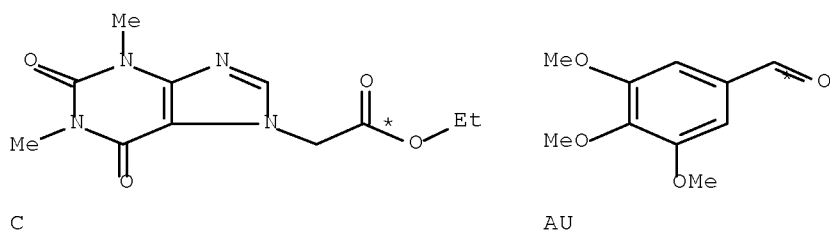
```

RX(103) OF 139 COMPOSED OF RX(2), RX(22), RX(29), RX(15)
RX(103)  C  +  AU  +  J  +  AJ  ==>  AM

```



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YIELD 64%

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(22) RCT F 41838-25-9, AU 86-81-7

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5

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CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

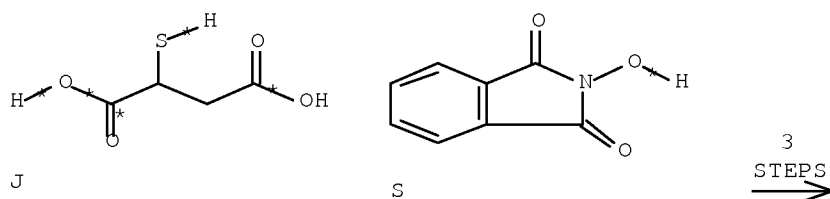
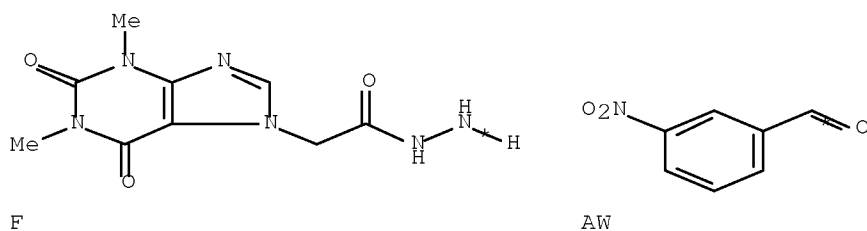
PRO AV 901781-63-3  
NTE intermediate was isolated

RX(29) RCT AV 901781-63-3  
RGT Q 7719-09-7 SOCl2  
PRO X 901781-70-2  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(15) RCT X 901781-70-2, AJ 6066-82-6  
RGT U 121-44-8 Et3N  
PRO AM 901781-56-4  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

RX(104) OF 139 COMPOSED OF RX(23), RX(30), RX(8)

RX(104) F + AW + J + S ==> AA



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(23) RCT F 41838-25-9, AW 99-61-6

STAGE(1)  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

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STAGE(2)

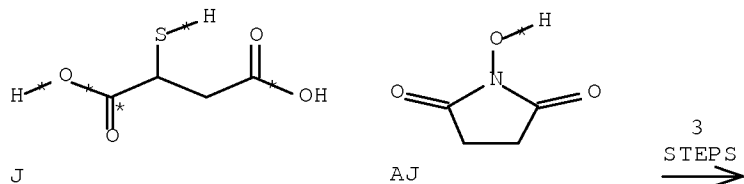
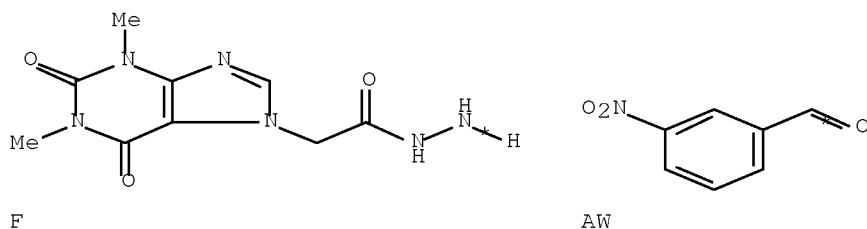
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO AX 901781-64-4  
NTE intermediate was isolated

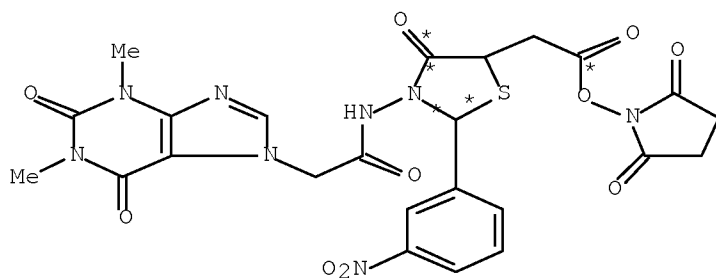
RX(30) RCT AX 901781-64-4  
RGT Q 7719-09-7 SOCl2  
PRO Z 901781-71-3  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(8) RCT Z 901781-71-3, S 524-38-9  
RGT U 121-44-8 Et3N  
PRO AA 901781-49-5  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

RX(105) OF 139 COMPOSED OF RX(23), RX(30), RX(16)  
RX(105) F + AW + J + AJ ==> AN



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AN  
YIELD 73%

RX(23) RCT F 41838-25-9, AW 99-61-6

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

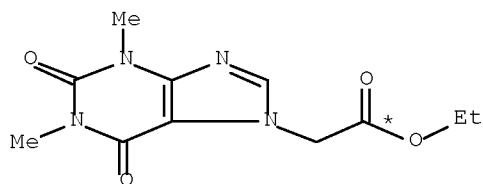
PRO AX 901781-64-4  
NTE intermediate was isolated

RX(30) RCT AX 901781-64-4  
RGT Q 7719-09-7 SOCl2  
PRO Z 901781-71-3  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

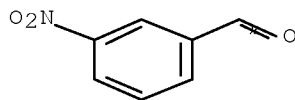
RX(16) RCT Z 901781-71-3, AJ 6066-82-6  
RGT U 121-44-8 Et3N  
PRO AN 901781-57-5  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

RX(106) OF 139 COMPOSED OF RX(2), RX(23), RX(30), RX(8)

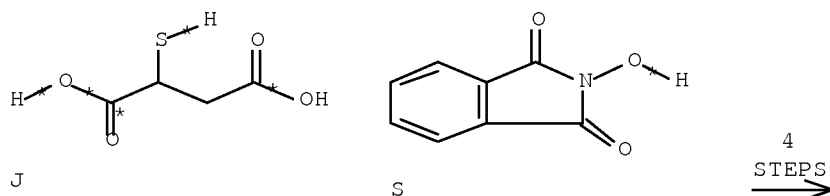
RX(106) C + AW + J + S ==> AA



C



AW



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

```

RX(2)      RCT  C 7029-96-1
           RGT  G 7803-57-8 N2H4-H2O
           PRO  F 41838-25-9
           SOL  123-91-1 Dioxane
           CON  6 hours, reflux

RX(23)     RCT  F 41838-25-9, AW 99-61-6

           STAGE(1)
             CAT  64-19-7 AcOH
             SOL  64-17-5 EtOH
             CON  5 hours, reflux

           STAGE(2)
             RCT  J 70-49-5
             CAT  7646-85-7 ZnCl2
             SOL  109-99-9 THF
             CON  10 hours, reflux

           PRO  AX 901781-64-4
           NTE  intermediate was isolated

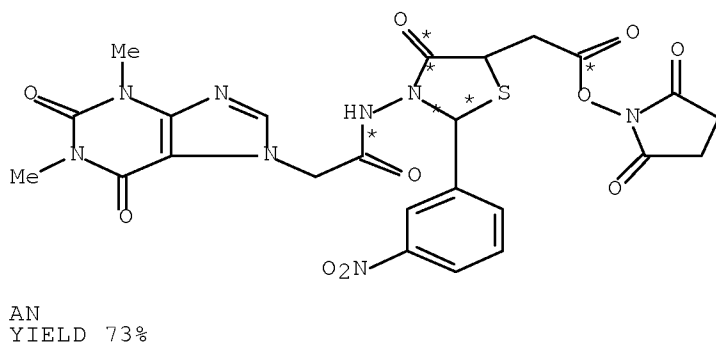
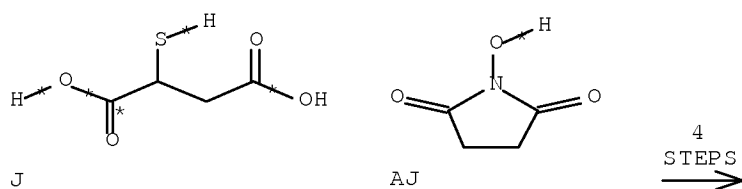
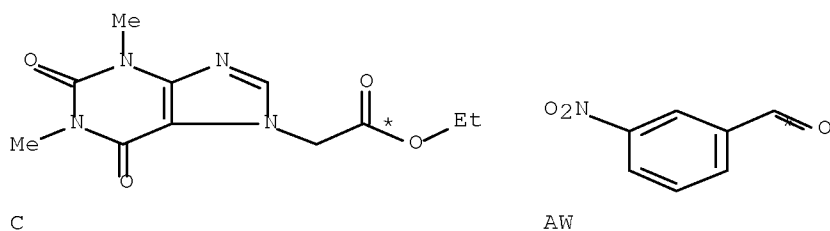
RX(30)     RCT  AX 901781-64-4
           RGT  Q 7719-09-7 SOCl2
           PRO  Z 901781-71-3
           SOL  108-88-3 PhMe
           CON  30 minutes, reflux

RX(8)      RCT  Z 901781-71-3, S 524-38-9
           RGT  U 121-44-8 Et3N
           PRO  AA 901781-49-5
           SOL  68-12-2 DMF
           CON  6 hours, room temperature
  
```

```

RX(107) OF 139 COMPOSED OF RX(2), RX(23), RX(30), RX(16)
RX(107)  C  +  AW  +  J  +  AJ  ==>  AN
  
```

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RX(2) RCT C 7029-96-1  
 RGT G 7803-57-8 N2H4-H2O  
 PRO F 41838-25-9  
 SOL 123-91-1 Dioxane  
 CON 6 hours, reflux

RX(23) RCT F 41838-25-9, AW 99-61-6

STAGE(1)

CAT 64-19-7 AcOH  
 SOL 64-17-5 EtOH  
 CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5  
 CAT 7646-85-7 ZnCl2

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SOL 109-99-9 THF  
CON 10 hours, reflux

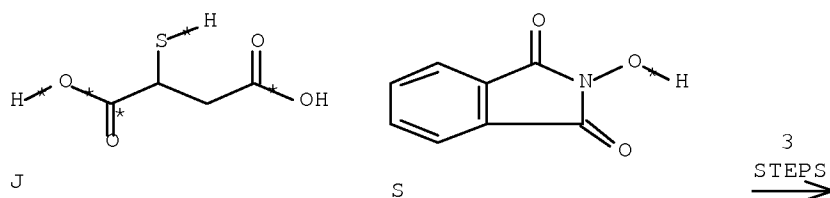
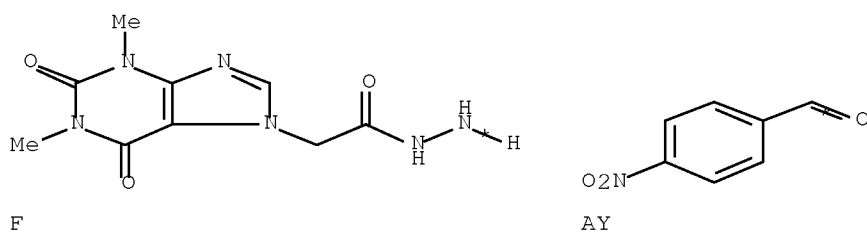
PRO AX 901781-64-4  
NTE intermediate was isolated

RX(30) RCT AX 901781-64-4  
RGT Q 7719-09-7 SOCl<sub>2</sub>  
PRO Z 901781-71-3  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(16) RCT Z 901781-71-3, AJ 6066-82-6  
RGT U 121-44-8 Et<sub>3</sub>N  
PRO AN 901781-57-5  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

RX(108) OF 139 COMPOSED OF RX(24), RX(31), RX(9)

RX(108) F + AY + J + S ==> AC



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(24) RCT F 41838-25-9, AY 555-16-8

STAGE(1)  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

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STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

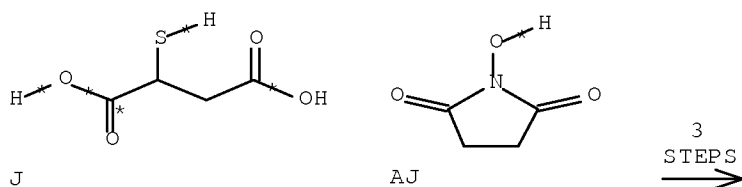
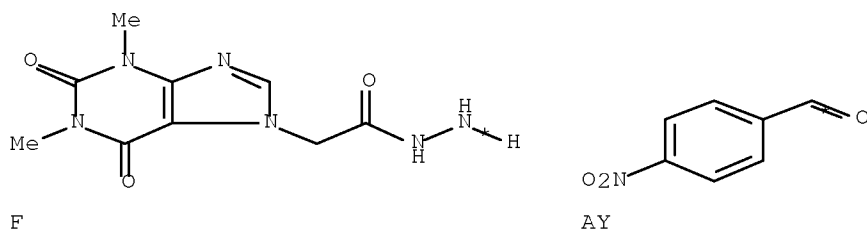
PRO AZ 901781-65-5  
NTE intermediate was isolated

RX(31) RCT AZ 901781-65-5  
RGT Q 7719-09-7 SOCl2  
PRO AB 901781-72-4  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(9) RCT AB 901781-72-4, S 524-38-9  
RGT U 121-44-8 Et3N  
PRO AC 901781-50-8  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

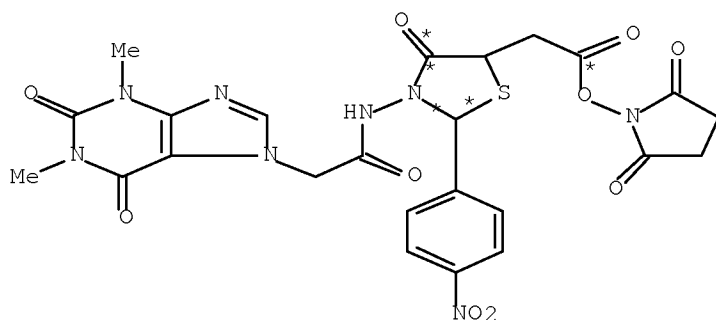
RX(109) OF 139 COMPOSED OF RX(24), RX(31), RX(17)

RX(109) F + AY + J + AJ ==> AO





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AO  
YIELD 69%

RX(24) RCT F 41838-25-9, AY 555-16-8

STAGE (1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE (2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

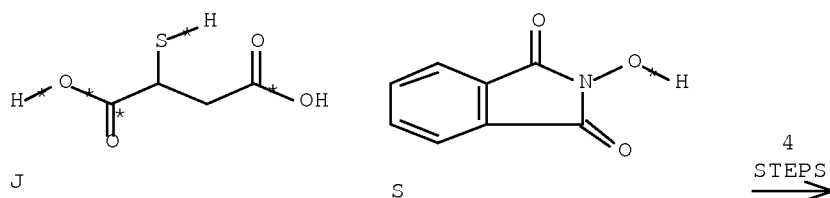
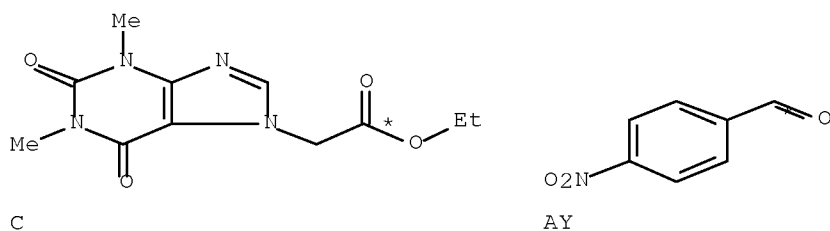
PRO AZ 901781-65-5  
NTE intermediate was isolated

RX(31)	RCT	AZ 901781-65-5
	RGT	Q 7719-09-7 SOC12
	PRO	AB 901781-72-4
	SOL	108-88-3 PhMe
	CON	30 minutes, reflux

RX(17)      RCT   AB 901781-72-4, AJ 6066-82-6  
              RGT   U 121-44-8 Et3N  
              PRO   AO 901781-58-6  
              SOL   68-12-2 DMF  
              CON   6 hours, room temperature

RX(110) OF 139 COMPOSED OF RX(2), RX(24), RX(31), RX(9)  
 RX(110) C + AY + J + S ==> AC

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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT C 7029-96-1  
 RGT G 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
 PRO F 41838-25-9  
 SOL 123-91-1 Dioxane  
 CON 6 hours, reflux

RX(24) RCT F 41838-25-9, AY 555-16-8

STAGE(1)

CAT 64-19-7 AcOH  
 SOL 64-17-5 EtOH  
 CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5  
 CAT 7646-85-7 ZnCl<sub>2</sub>  
 SOL 109-99-9 THF  
 CON 10 hours, reflux

PRO AZ 901781-65-5  
 NTE intermediate was isolated

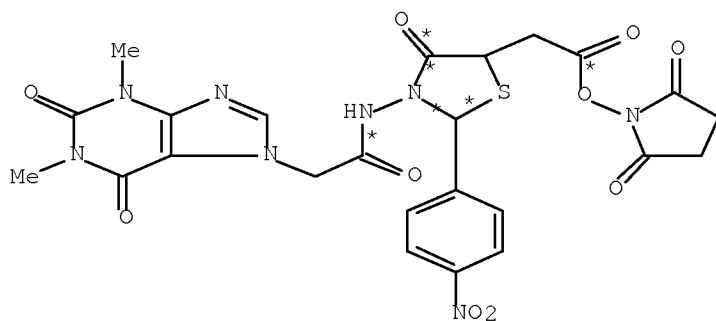
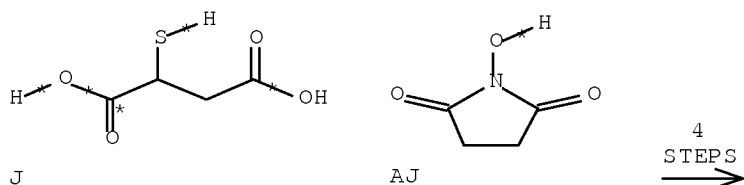
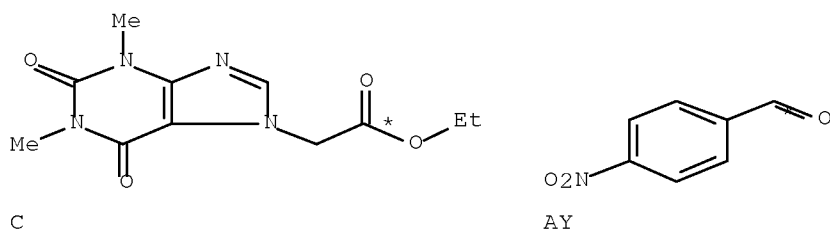
RX(31) RCT AZ 901781-65-5  
 RGT Q 7719-09-7 SOCl<sub>2</sub>  
 PRO AB 901781-72-4  
 SOL 108-88-3 PhMe  
 CON 30 minutes, reflux

RX(9) RCT AB 901781-72-4, S 524-38-9  
 RGT U 121-44-8 Et<sub>3</sub>N

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PRO AC 901781-50-8  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

RX(111) OF 139 COMPOSED OF RX(2), RX(24), RX(31), RX(17)  
RX(111) C + AY + J + AJ ==> AO



AO  
YIELD 69%

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

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RX(24) RCT F 41838-25-9, AY 555-16-8

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

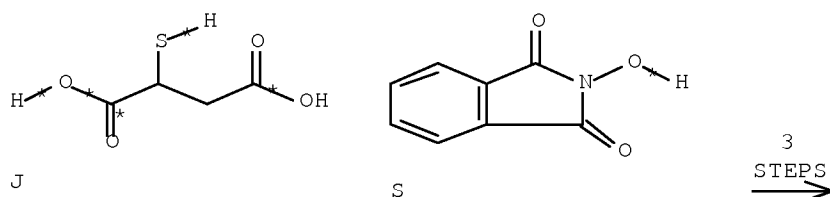
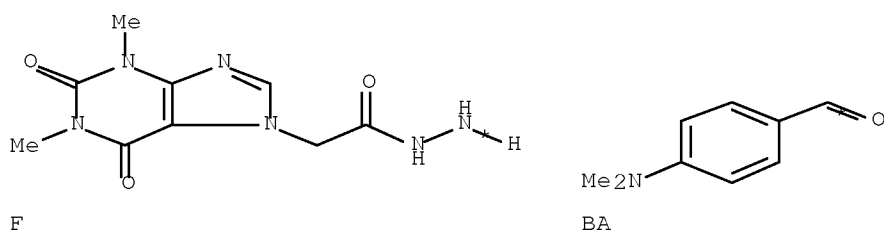
PRO AZ 901781-65-5  
NTE intermediate was isolated

RX(31) RCT AZ 901781-65-5  
RGT Q 7719-09-7 SOCl2  
PRO AB 901781-72-4  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(17) RCT AB 901781-72-4, AJ 6066-82-6  
RGT U 121-44-8 Et3N  
PRO AO 901781-58-6  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

RX(112) OF 139 COMPOSED OF RX(25), RX(32), RX(10)

RX(112) F + BA + J + S ==> AE



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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(25) RCT F 41838-25-9, BA 100-10-7

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

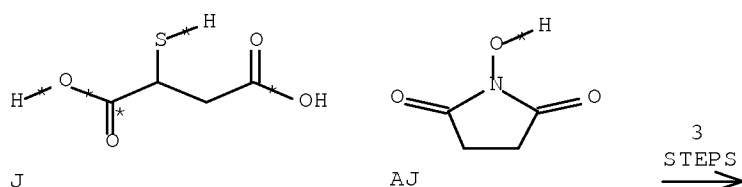
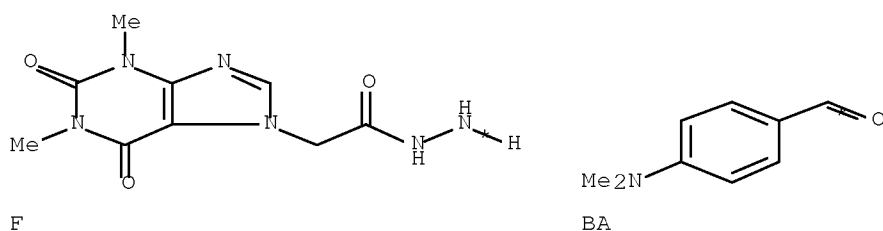
PRO BB 901781-66-6  
NTE intermediate was isolated

RX(32) RCT BB 901781-66-6  
RGT Q 7719-09-7 SOCl2  
PRO AD 901781-73-5  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

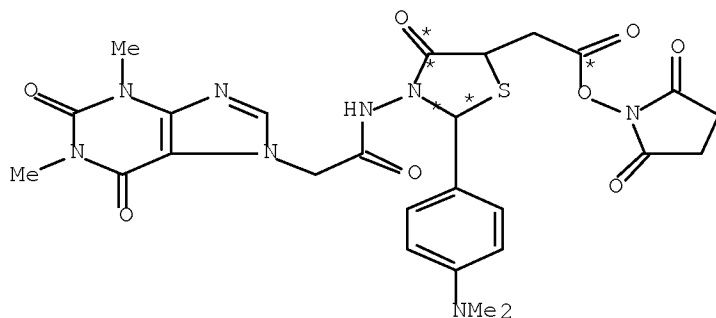
RX(10) RCT AD 901781-73-5, S 524-38-9  
RGT U 121-44-8 Et3N  
PRO AE 901781-51-9  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

RX(113) OF 139 COMPOSED OF RX(25), RX(32), RX(18)

RX(113) F + BA + J + AJ ==> AF



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AP  
YIELD 62%

RX(25) RCT F 41838-25-9, BA 100-10-7

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

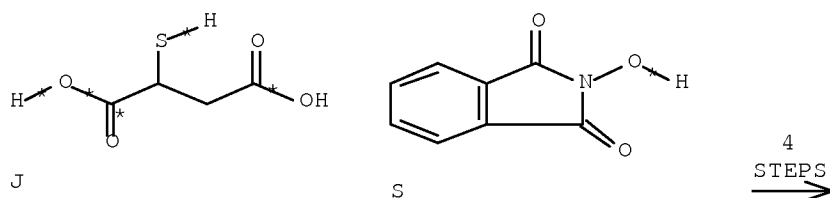
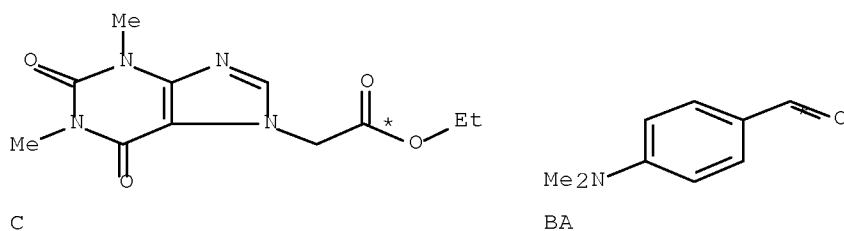
PRO BB 901781-66-6  
NTE intermediate was isolated

RX(32) RCT BB 901781-66-6  
RGT Q 7719-09-7 SOCl2  
PRO AD 901781-73-5  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(18) RCT AD 901781-73-5, AJ 6066-82-6  
RGT U 121-44-8 Et3N  
PRO AP 901781-59-7  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

RX(114) OF 139 COMPOSED OF RX(2), RX(25), RX(32), RX(10)  
RX(114) C + BA + J + S ==> AE

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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(25) RCT F 41838-25-9, BA 100-10-7

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO BB 901781-66-6  
NTE intermediate was isolated

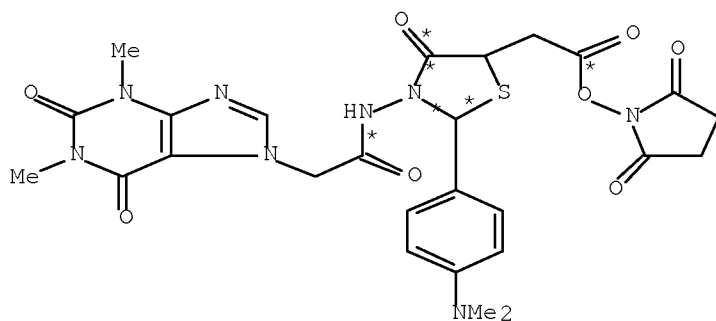
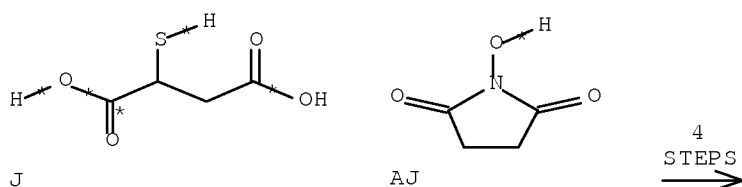
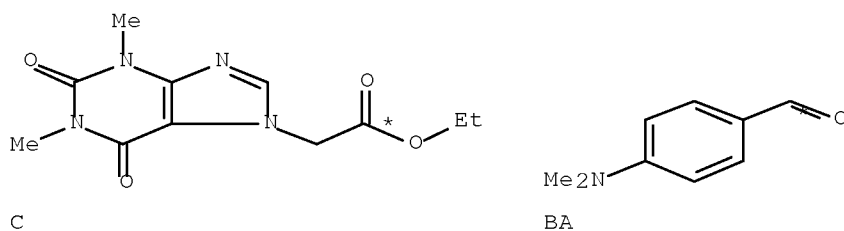
RX(32) RCT BB 901781-66-6  
RGT Q 7719-09-7 SOCl2  
PRO AD 901781-73-5  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(10) RCT AD 901781-73-5, S 524-38-9  
RGT U 121-44-8 Et3N

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PRO AE 901781-51-9  
 SOL 68-12-2 DMF  
 CON 6 hours, room temperature

RX(115) OF 139 COMPOSED OF RX(2), RX(25), RX(32), RX(18)  
 RX(115) C + BA + J + AJ ==> AP



AP  
 YIELD 62%

RX(2) RCT C 7029-96-1  
 RGT G 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
 PRO F 41838-25-9  
 SOL 123-91-1 Dioxane  
 CON 6 hours, reflux



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RX(25) RCT F 41838-25-9, BA 100-10-7

STAGE(1)

CAT 64-19-7 AcOH

SOL 64-17-5 EtOH

CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5

CAT 7646-85-7 ZnCl<sub>2</sub>

SOL 109-99-9 THF

CON 10 hours, reflux

PRO BB 901781-66-6

NTE intermediate was isolated

RX(32) RCT BB 901781-66-6

RGT Q 7719-09-7 SOCl<sub>2</sub>

PRO AD 901781-73-5

SOL 108-88-3 PhMe

CON 30 minutes, reflux

RX(18) RCT AD 901781-73-5, AJ 6066-82-6

RGT U 121-44-8 Et<sub>3</sub>N

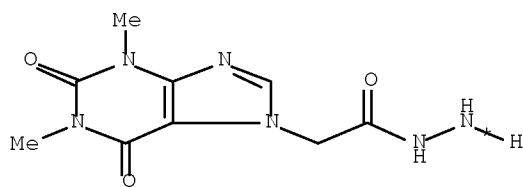
PRO AP 901781-59-7

SOL 68-12-2 DMF

CON 6 hours, room temperature

RX(116) OF 139 COMPOSED OF RX(26), RX(33), RX(11)

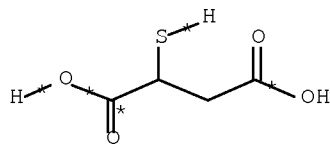
RX(116) F + BC + J + S ==> AG



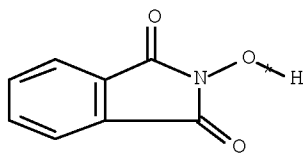
F



BC



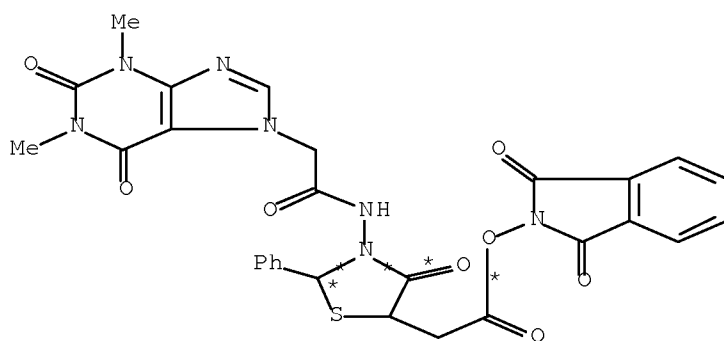
J



S

3  
STEPS  
→

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AG  
YIELD 60%

RX(26) RCT F 41838-25-9, BC 100-52-7

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl<sub>2</sub>  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO BD 901781-67-7  
NTE intermediate was isolated

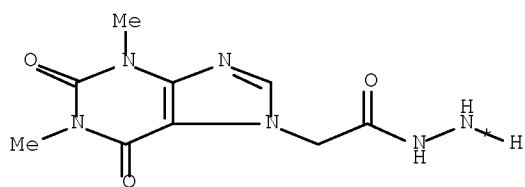
RX(33) RCT BD 901781-67-7  
RGT Q 7719-09-7 SOCl<sub>2</sub>  
PRO AF 901781-74-6  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(11) RCT AF 901781-74-6, S 524-38-9  
RGT U 121-44-8 Et<sub>3</sub>N  
PRO AG 901781-52-0  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

RX(117) OF 139 COMPOSED OF RX(26), RX(33), RX(19)

RX(117) F + BC + J + AJ ==> AQ

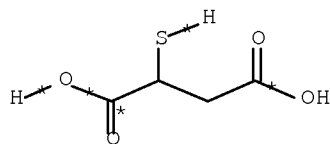
10/595943



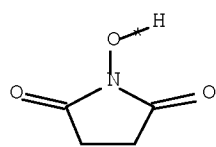
F



BC

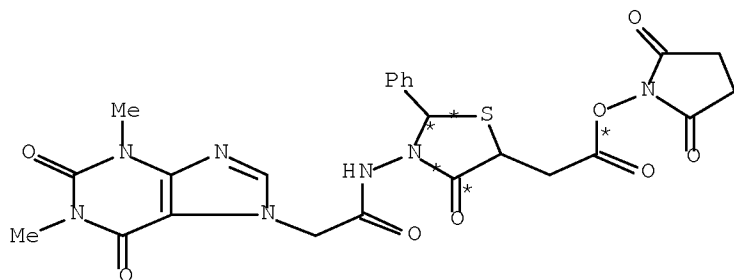


J



AJ

3  
STEPS  
→



AQ  
YIELD 68%

RX(26) RCT F 41838-25-9, BC 100-52-7

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

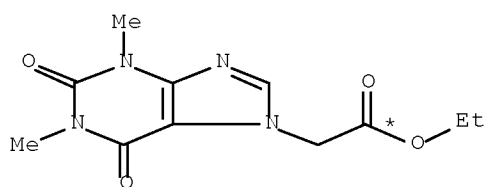
PRO BD 901781-67-7  
NTE intermediate was isolated

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RX(33) RCT BD 901781-67-7  
 RGT Q 7719-09-7 SOCl2  
 PRO AF 901781-74-6  
 SOL 108-88-3 PhMe  
 CON 30 minutes, reflux

RX(19) RCT AF 901781-74-6, AJ 6066-82-6  
 RGT U 121-44-8 Et3N  
 PRO AQ 901781-60-0  
 SOL 68-12-2 DMF  
 CON 6 hours, room temperature

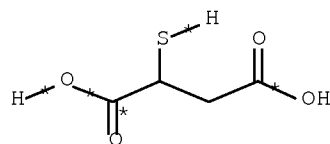
RX(118) OF 139 COMPOSED OF RX(2), RX(26), RX(33), RX(11)  
 RX(118) C + BC + J + S ==> AG



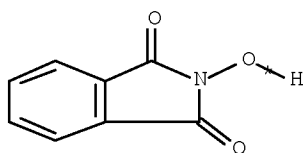
C



BC

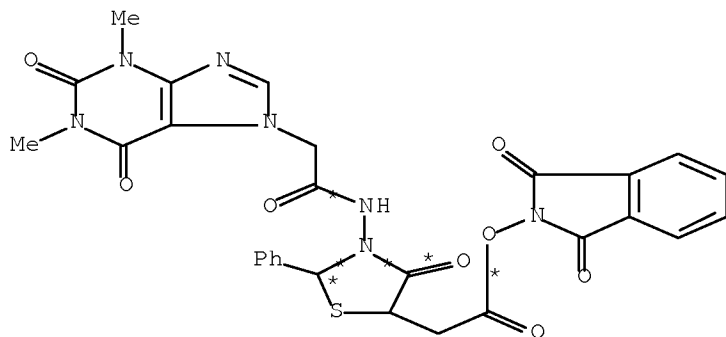


J



S

4  
STEPS  
→



AG  
YIELD 60%

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RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(26) RCT F 41838-25-9, BC 100-52-7

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

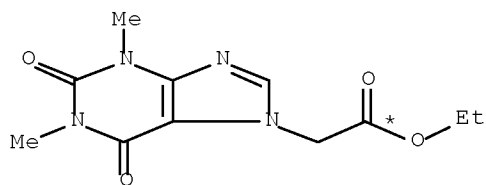
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO BD 901781-67-7  
NTE intermediate was isolated

RX(33) RCT BD 901781-67-7  
RGT Q 7719-09-7 SOCl2  
PRO AF 901781-74-6  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(11) RCT AF 901781-74-6, S 524-38-9  
RGT U 121-44-8 Et3N  
PRO AG 901781-52-0  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

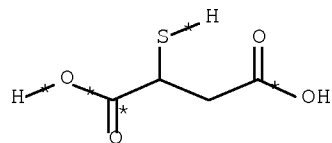
RX(119) OF 139 COMPOSED OF RX(2), RX(26), RX(33), RX(19)  
RX(119) C + BC + J + AJ ==> AQ



C

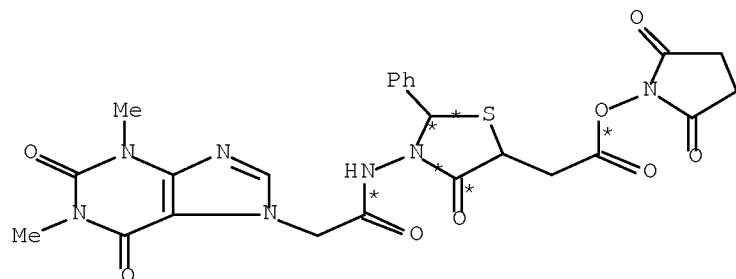
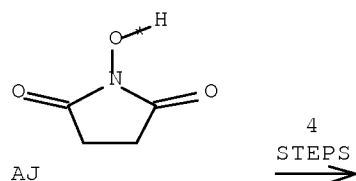


BC



J

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AQ  
YIELD 68%

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(26) RCT F 41838-25-9, BC 100-52-7

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO BD 901781-67-7  
NTE intermediate was isolated

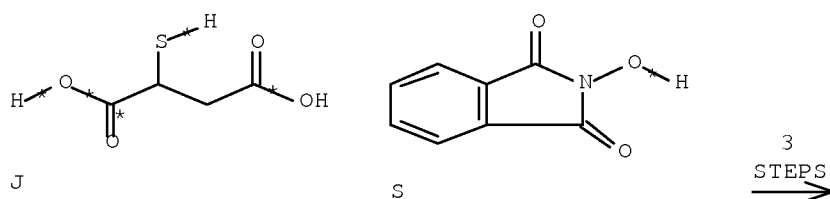
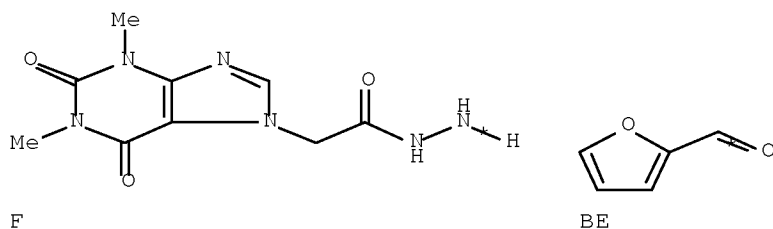
RX(33) RCT BD 901781-67-7  
RGT Q 7719-09-7 SOCl2  
PRO AF 901781-74-6  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(19) RCT AF 901781-74-6, AJ 6066-82-6  
RGT U 121-44-8 Et3N  
PRO AQ 901781-60-0

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SOL 68-12-2 DMF  
CON 6 hours, room temperature

RX(120) OF 139 COMPOSED OF RX(27), RX(34), RX(12)  
RX(120) F + BE + J + S ==> AI



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(27) RCT F 41838-25-9, BE 98-01-1

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

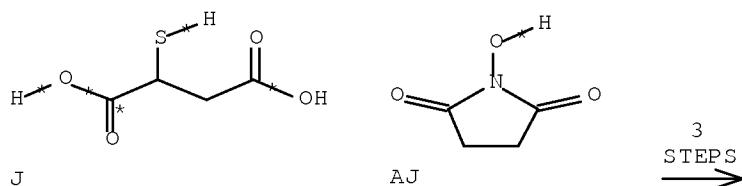
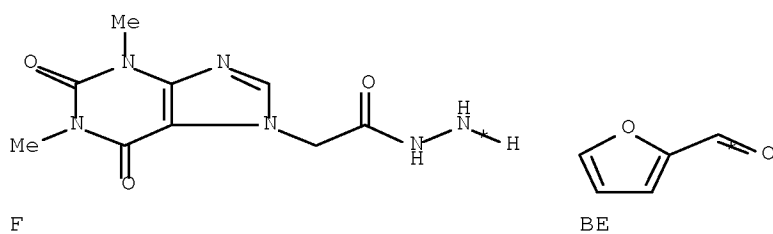
PRO BF 901781-68-8  
NTE intermediate was isolated

RX(34) RCT BF 901781-68-8  
RGT Q 7719-09-7 SOCl2  
PRO AH 901781-75-7  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

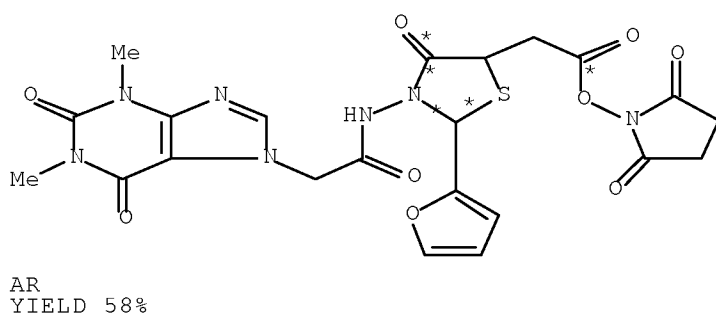
10/595943

RX(12) RCT AH 901781-75-7, S 524-38-9  
 RGT U 121-44-8 Et3N  
 PRO AI 901781-53-1  
 SOL 68-12-2 DMF  
 CON 6 hours, room temperature

RX(121) OF 139 COMPOSED OF RX(27), RX(34), RX(20)  
 RX(121) F + BE + J + AJ ==> AR



3  
STEPS  
→



AR  
 YIELD 58%

RX(27) RCT F 41838-25-9, BE 98-01-1

STAGE(1)

CAT 64-19-7 AcOH  
 SOL 64-17-5 EtOH  
 CON 5 hours, reflux



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STAGE(2)

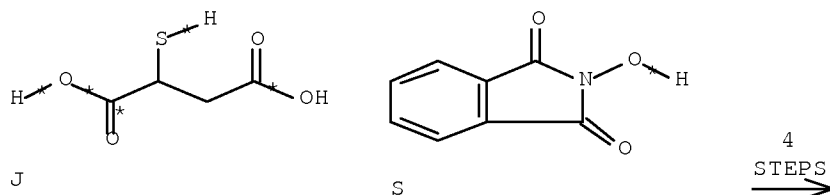
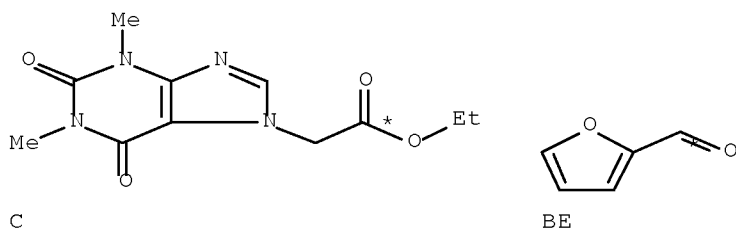
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO BF 901781-68-8  
NTE intermediate was isolated

RX(34) RCT BF 901781-68-8  
RGT Q 7719-09-7 SOCl2  
PRO AH 901781-75-7  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(20) RCT AH 901781-75-7, AJ 6066-82-6  
RGT U 121-44-8 Et3N  
PRO AR 901781-61-1  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

RX(122) OF 139 COMPOSED OF RX(2), RX(27), RX(34), RX(12)  
RX(122) C + BE + J + S ==> AI



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9

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SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(27) RCT F 41838-25-9, BE 98-01-1

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

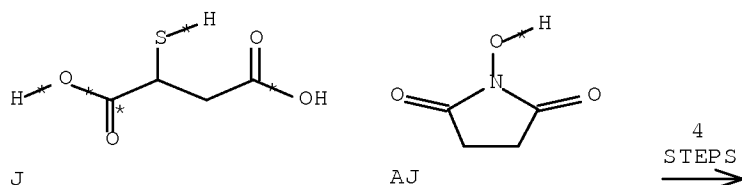
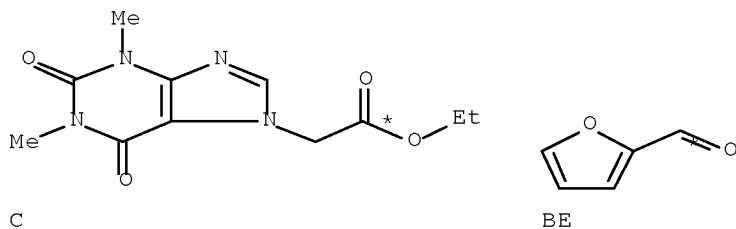
RCT J 76-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO BF 901781-68-8  
NTE intermediate was isolated

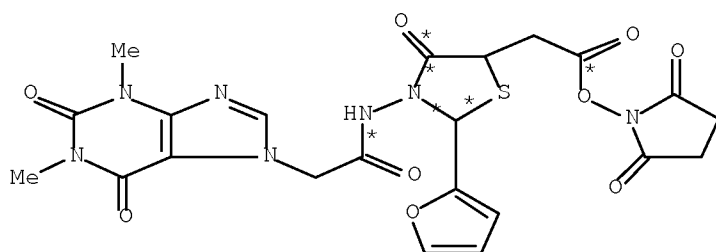
RX(34) RCT BF 901781-68-8  
RGT Q 7719-09-7 SOCl2  
PRO AH 901781-75-7  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(12) RCT AH 901781-75-7, S 524-38-9  
RGT U 121-44-8 Et3N  
PRO AI 901781-53-1  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

RX(123) OF 139 COMPOSED OF RX(2), RX(27), RX(34), RX(20)  
RX(123) C + BE + J + AJ ==> AR



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AR  
YIELD 58%

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(27) RCT F 41838-25-9, BE 98-01-1

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

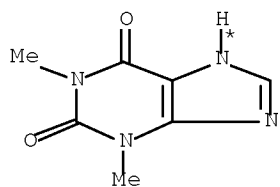
PRO BF 901781-68-8  
NTE intermediate was isolated

RX(34) RCT BF 901781-68-8  
RGT Q 7719-09-7 SOCl2  
PRO AH 901781-75-7  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

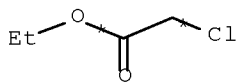
RX(20) RCT AH 901781-75-7, AJ 6066-82-6  
RGT U 121-44-8 Et3N  
PRO AR 901781-61-1  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

RX(124) OF 139 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5)  
RX(124) A + B + I + J + S ==> T

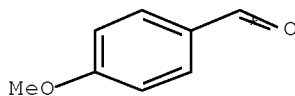
10/595943



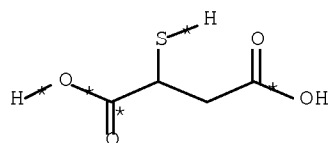
A



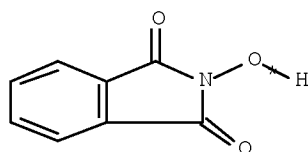
B



I



J



S

5  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5

CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1

RGT G 7803-57-8 N2H4-H2O

PRO F 41838-25-9

SOL 123-91-1 Dioxane

CON 6 hours, reflux

RX(3) RCT F 41838-25-9, I 123-11-5

STAGE(1)

CAT 64-19-7 AcOH

SOL 64-17-5 EtOH

CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5

CAT 7646-85-7 ZnCl2

SOL 109-99-9 THF

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CON 10 hours, reflux

PRO K 901781-44-0

NTE intermediate was isolated

RX(4) RCT K 901781-44-0

RGT Q 7719-09-7 SOCl<sub>2</sub>

PRO P 901781-45-1

SOL 108-88-3 PhMe

CON 30 minutes, reflux

RX(5) RCT P 901781-45-1, S 524-38-9

RGT U 121-44-8 Et<sub>3</sub>N

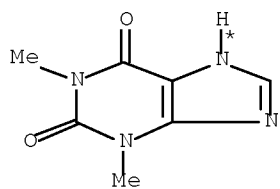
PRO T 901781-46-2

SOL 68-12-2 DMF

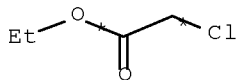
CON 6 hours, room temperature

RX(125) OF 139 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(13)

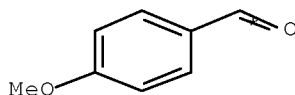
RX(125) A + B + I + J + AJ ==> AK



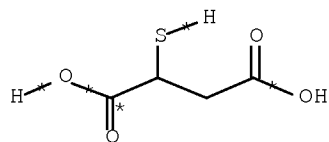
A



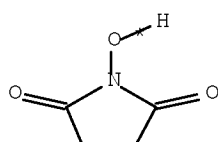
B



I



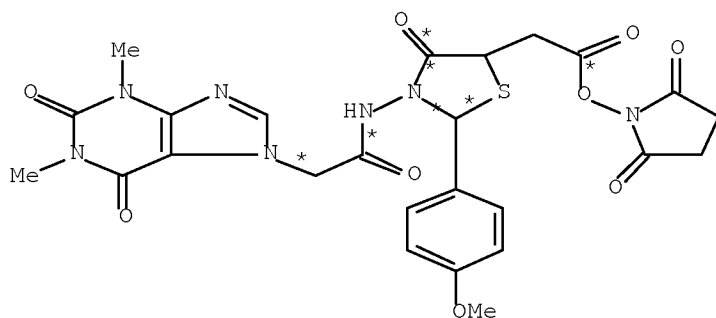
J



AJ

5  
STEPS  
→

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AK  
YIELD 70%

RX(1) RCT A 58-55-9  
STAGE(1)  
RGT D 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

STAGE(2)  
RCT B 105-39-5  
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(3) RCT F 41838-25-9, I 123-11-5

STAGE(1)  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)  
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO K 901781-44-0  
NTE intermediate was isolated

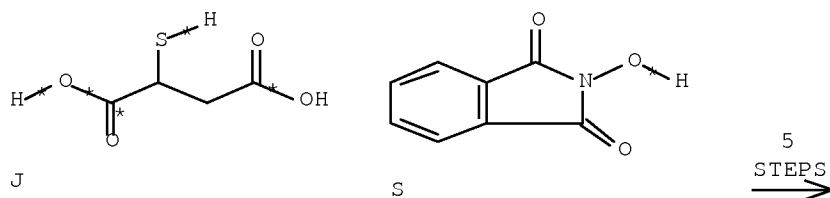
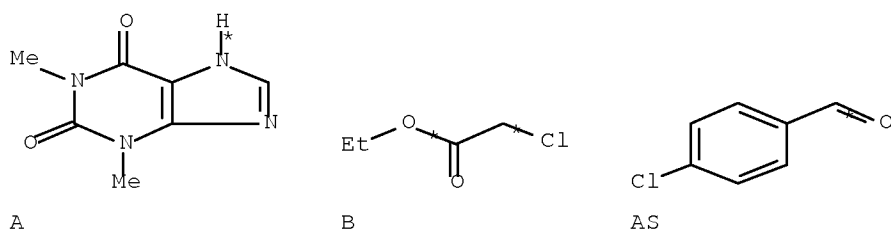
RX(4) RCT K 901781-44-0  
RGT Q 7719-09-7 SOCl2  
PRO P 901781-45-1  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(13) RCT P 901781-45-1, AJ 6066-82-6

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RGT U 121-44-8 Et3N  
 PRO AK 901781-54-2  
 SOL 68-12-2 DMF  
 CON 6 hours, room temperature

RX(126) OF 139 COMPOSED OF RX(1), RX(2), RX(21), RX(28), RX(6)  
 RX(126) A + B + AS + J + S ==> W



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH  
 SOL 68-12-2 DMF  
 CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5  
 CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
 RGT G 7803-57-8 N2H4-H2O  
 PRO F 41838-25-9  
 SOL 123-91-1 Dioxane  
 CON 6 hours, reflux

RX(21) RCT F 41838-25-9, AS 104-88-1

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STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

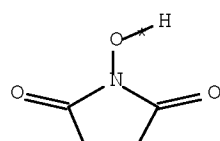
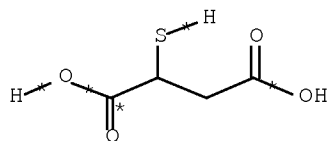
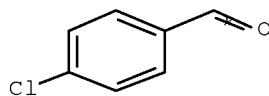
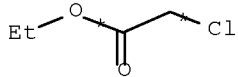
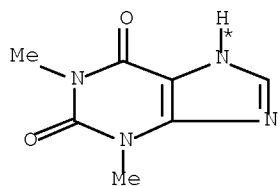
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO AT 901781-62-2  
NTE intermediate was isolated

RX(28) RCT AT 901781-62-2  
RGT Q 7719-09-7 SOCl2  
PRO V 901781-69-9  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(6) RCT V 901781-69-9, S 524-38-9  
RGT U 121-44-8 Et3N  
PRO W 901781-47-3  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

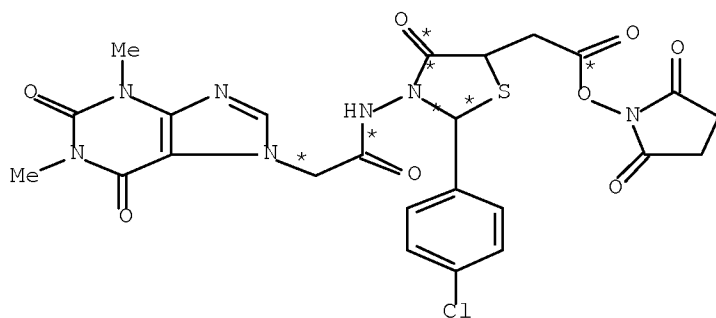
RX(127) OF 139 COMPOSED OF RX(1), RX(2), RX(21), RX(28), RX(14)  
RX(127) A + B + AS + J + AJ ==> AL



5  
STEPS  
→



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AL  
YIELD 62%

```

RX(1)      RCT   A 58-55-9

          STAGE(1)
            RGT   D 7646-69-7 NaH
            SOL   68-12-2 DMF
            CON   2 hours, room temperature

```

```
STAGE(2)
      RCT  B 105-39-5
      CON  6 hours, reflux
```

PRO C 7029-96-1

RX (2)            RCT   C 7029-96-1  
                  RGT   G ~~7803-57-8~~ N2H4-H2O  
                  PRO   F 41838-25-9  
                  SOL   123-91-1 Dioxane  
                  CON   6 hours, reflux

RX(21) RCT F 41838-25-9, AS 104-88-1

```
STAGE(1)
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux
```

STAGE (2)

RCT	J 70-49-5	
CAT	7646-85-7	ZnCl <sub>2</sub>
SOL	109-99-9	THF
CON	10 hours,	reflux

PRO AT 901781-62-2  
NTE intermediate was isolated

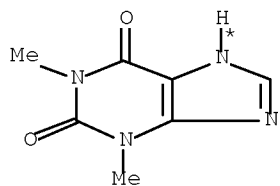
RX(28)      RCT    AT 901781-62-2  
              RGT    Q 7719-09-7 SOC12  
              PRO    V 901781-69-9  
              SOL    108-88-3 PhMe  
              CON    30 minutes, reflux

RX(14) RCT V 901781-69-9, AJ 6066-82-6

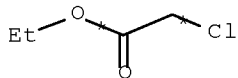
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RGT U 121-44-8 Et3N  
PRO AL 901781-55-3  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

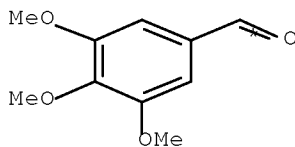
RX(128) OF 139 COMPOSED OF RX(1), RX(2), RX(22), RX(29), RX(7)  
RX(128) A + B + AU + J + S ==> Y



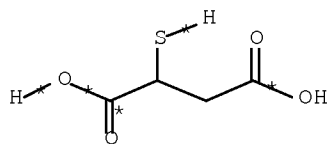
A



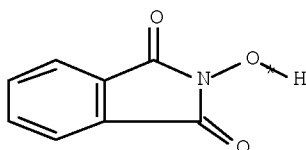
B



AU



J



S

5  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5  
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(22) RCT F 41838-25-9, AU 86-81-7

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STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

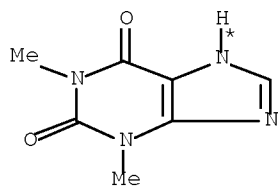
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO AV 901781-63-3  
NTE intermediate was isolated

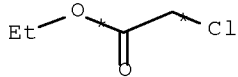
RX(29) RCT AV 901781-63-3  
RGT Q 7719-09-7 SOCl2  
PRO X 901781-70-2  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(7) RCT X 901781-70-2, S 524-38-9  
RGT U 121-44-8 Et3N  
PRO Y 901781-48-4  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

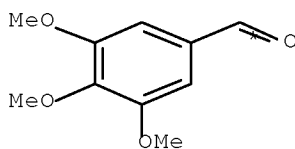
RX(129) OF 139 COMPOSED OF RX(1), RX(2), RX(22), RX(29), RX(15)  
RX(129) A + B + AU + J + AJ ==> AM



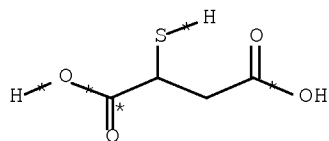
A



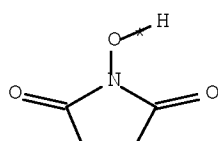
B



AU



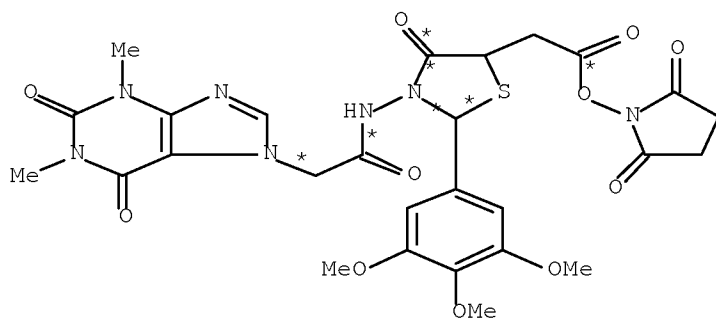
J



AJ

5  
STEPS  
→

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AM  
YIELD 64%

RX(1) RCT A 58-55-9  
STAGE(1)  
RGT D 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

STAGE(2)  
RCT B 105-39-5  
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(22) RCT F 41838-25-9, AU 86-81-7

STAGE(1)  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)  
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO AV 901781-63-3  
NTE intermediate was isolated

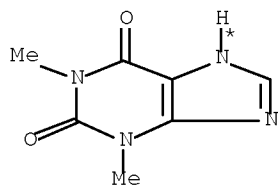
RX(29) RCT AV 901781-63-3  
RGT Q 7719-09-7 SOCl2  
PRO X 901781-70-2  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(15) RCT X 901781-70-2, AJ 6066-82-6

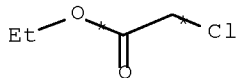
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RGT U 121-44-8 Et3N  
PRO AM 901781-56-4  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

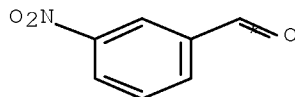
RX(130) OF 139 COMPOSED OF RX(1), RX(2), RX(23), RX(30), RX(8)  
RX(130) A + B + AW + J + S ==> AA



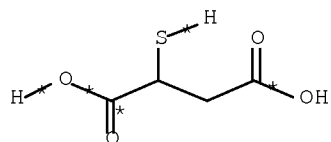
A



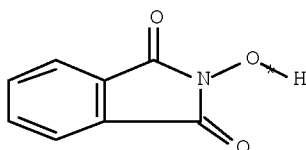
B



AW



J



S

5  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5  
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(23) RCT F 41838-25-9, AW 99-61-6

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STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

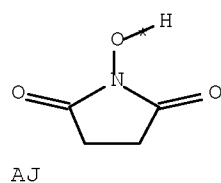
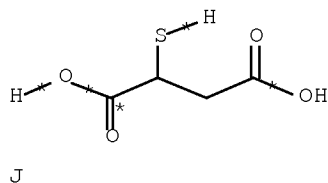
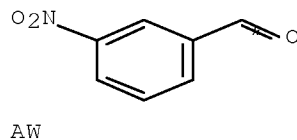
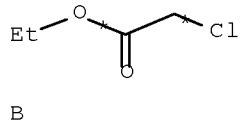
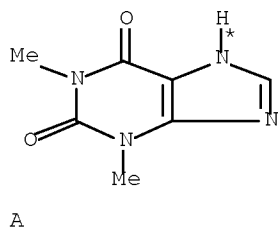
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO AX 901781-64-4  
NTE intermediate was isolated

RX(30) RCT AX 901781-64-4  
RGT Q 7719-09-7 SOCl2  
PRO Z 901781-71-3  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

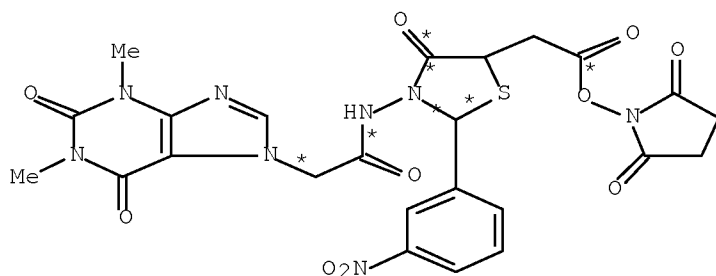
RX(8) RCT Z 901781-71-3, S 524-38-9  
RGT U 121-44-8 Et3N  
PRO AA 901781-49-5  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

RX(131) OF 139 COMPOSED OF RX(1), RX(2), RX(23), RX(30), RX(16)  
RX(131) A + B + AW + J + AJ ==> AN



5  
STEPS  
→

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AN  
YIELD 73%

```

RX(1)      RCT   A 58-55-9

              STAGE(1)
                RGT   D 7646-69-7 NaH
                SOL   68-12-2 DMF
                CON   2 hours, room temperature

```

```
STAGE(2)
  RCT  B 105-39-5
  CON  6 hours, reflux
```

PRO C 7029-96-1

RX (2)            RCT   C 7029-96-1  
                  RGT   G ~~7803-57-8~~ N2H4-H2O  
                  PRO   F 41838-25-9  
                  SOL   123-91-1 Dioxane  
                  CON   6 hours, reflux

RX(23)      RCT    F 41838-25-9, AW 99-61-6

```
STAGE(1)
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux
```

```
STAGE(2)
  RCT  J 70-49-5
  CAT  7646-85-7 ZnCl2
  SOL  109-99-9 THF
  CON  10 hours, reflux
```

PRO AX 901781-64-4  
NTE intermediate was isolated

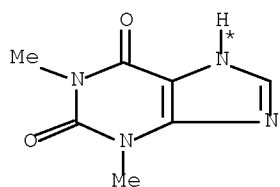
RX(30)	RCT	AX 901781-64-4
	RGT	Q 7719-09-7 SOC12
	PRO	Z 901781-71-3
	SOL	108-88-3 PhMe
	CON	30 minutes, reflux

RX(16)      RCT    Z 901781-71-3, AJ 6066-82-6  
               RGT    U 121-44-8 Et3N

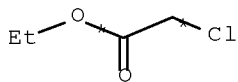
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PRO AN 901781-57-5  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

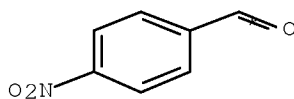
RX(132) OF 139 COMPOSED OF RX(1), RX(2), RX(24), RX(31), RX(9)  
RX(132) A + B + AY + J + S ==> AC



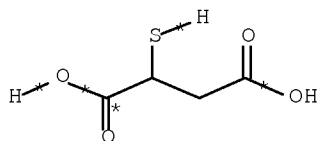
A



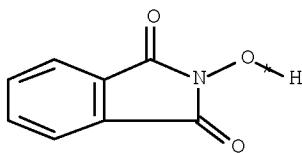
B



AY



J



S

5  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5  
CON 6 hours, reflux



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PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
RGT G ~~7803-57-8~~ N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(24) RCT F 41838-25-9, AY 555-16-8

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

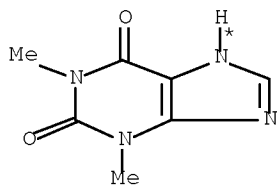
RCT J ~~70-49-5~~  
CAT ~~7646-85-7~~ ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO AZ 901781-65-5  
NTE intermediate was isolated

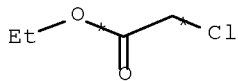
RX(31) RCT AZ 901781-65-5  
RGT Q 7719-09-7 SOCl2  
PRO AB 901781-72-4  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(9) RCT AB 901781-72-4, S 524-38-9  
RGT U 121-44-8 Et3N  
PRO AC ~~901781-50-8~~  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

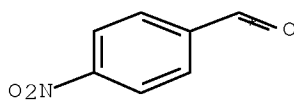
RX(133) OF 139 COMPOSED OF RX(1), RX(2), RX(24), RX(31), RX(17)  
RX(133) A + B + AY + J + AJ ==> AO



A

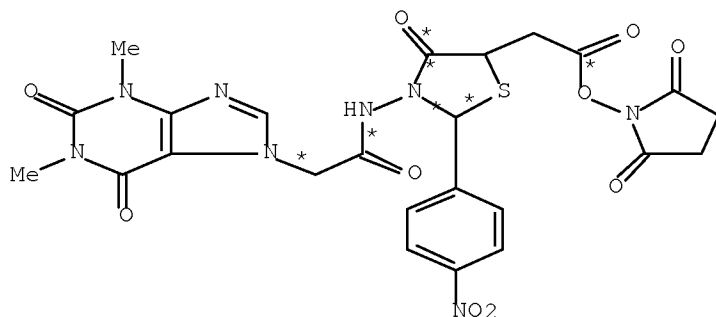
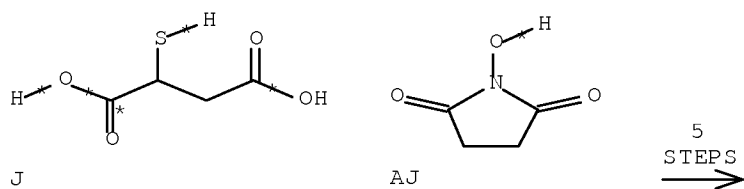


B



AY

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AO  
YIELD 69%

RX(1) RCT A 58-55-9  
STAGE(1)  
RGT D 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

STAGE(2)  
RCT B 105-39-5  
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(24) RCT F 41838-25-9, AY 555-16-8

STAGE(1)  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)  
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2

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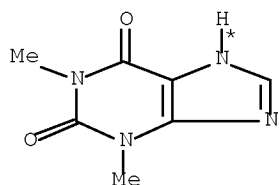
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO AZ 901781-65-5  
NTE intermediate was isolated

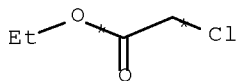
RX(31) RCT AZ 901781-65-5  
RGT Q 7719-09-7 SOCl<sub>2</sub>  
PRO AB 901781-72-4  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(17) RCT AB 901781-72-4, AJ 6066-82-6  
RGT U 121-44-8 Et<sub>3</sub>N  
PRO AO 901781-58-6  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

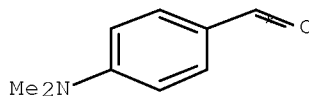
RX(134) OF 139 COMPOSED OF RX(1), RX(2), RX(25), RX(32), RX(10)  
RX(134) A + B + BA + J + S ==> AE



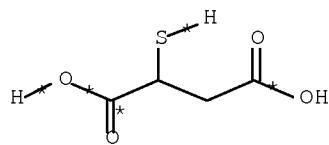
A



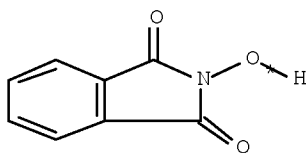
B



BA



J



S

5  
STEPS  
➔

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(1) RCT A 58-55-9

STAGE(1)  
RGT D 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

STAGE(2)

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RCT B 105-39-5  
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(25) RCT F 41838-25-9, BA 100-10-7

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

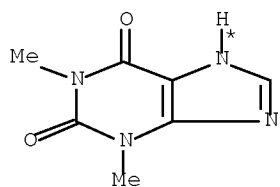
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO BB 901781-66-6  
NTE intermediate was isolated

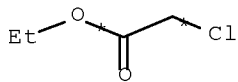
RX(32) RCT BB 901781-66-6  
RGT Q 7719-09-7 SOCl2  
PRO AD 901781-73-5  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(10) RCT AD 901781-73-5, S 524-38-9  
RGT U 121-44-8 Et3N  
PRO AE 901781-51-9  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

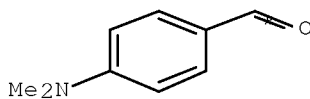
RX(135) OF 139 COMPOSED OF RX(1), RX(2), RX(25), RX(32), RX(18)  
RX(135) A + B + BA + J + AJ ==> AP



A

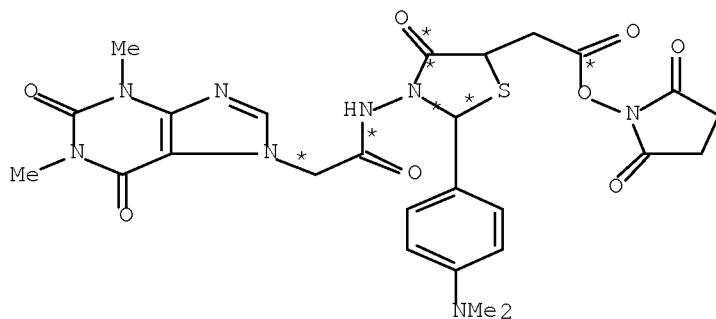
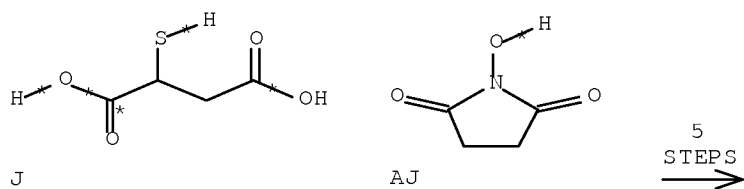


B



BA

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AP  
YIELD 62%

RX(1) RCT A 58-55-9  
STAGE(1)  
RGT D 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

STAGE(2)  
RCT B 105-39-5  
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(25) RCT F 41838-25-9, BA 100-10-7

STAGE(1)  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)  
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2

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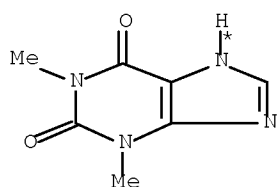
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO BB 901781-66-6  
NTE intermediate was isolated

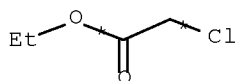
RX(32) RCT BB 901781-66-6  
RGT Q 7719-09-7 SOCl<sub>2</sub>  
PRO AD 901781-73-5  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(18) RCT AD 901781-73-5, AJ 6066-82-6  
RGT U 121-44-8 Et<sub>3</sub>N  
PRO AP 901781-59-7  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

RX(136) OF 139 COMPOSED OF RX(1), RX(2), RX(26), RX(33), RX(11)  
RX(136) A + B + BC + J + S ==> AG



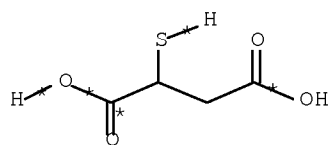
A



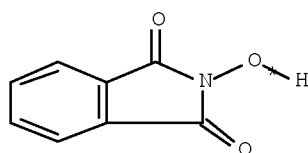
B



BC



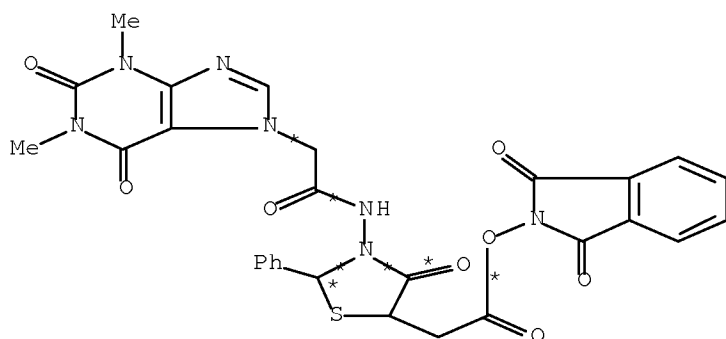
J



S

5  
STEPS  
→

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AG  
YIELD 60%

RX(1) RCT A 58-55-9  
STAGE(1)  
RGT D 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

STAGE(2)  
RCT B 105-39-5  
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
RGT G 7803-57-8 N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(26) RCT F 41838-25-9, BC 100-52-7

STAGE(1)  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)  
RCT J 70-49-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

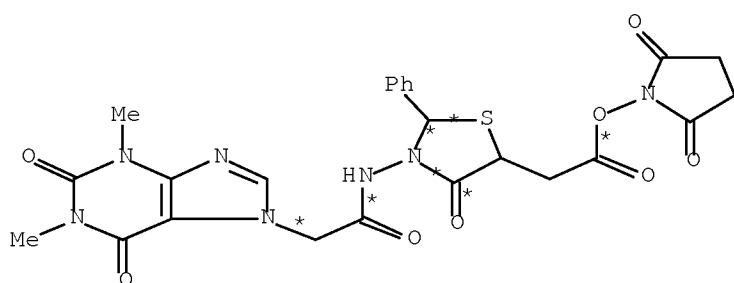
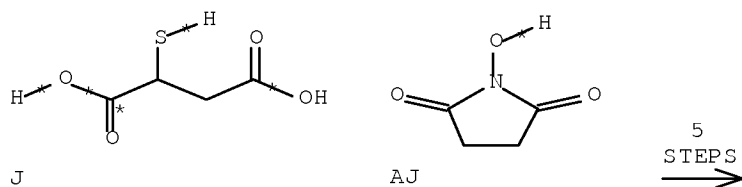
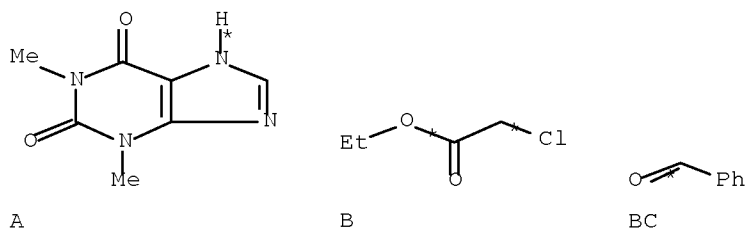
PRO BD 901781-67-7  
NTE intermediate was isolated

RX(33) RCT BD 901781-67-7  
RGT Q 7719-09-7 SOCl2  
PRO AF 901781-74-6  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

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RX(11) RCT AF 901781-74-6, S 524-38-9  
 RGT U 121-44-8 Et3N  
 PRO AG 901781-52-0  
 SOL 68-12-2 DMF  
 CON 6 hours, room temperature

RX(137) OF 139 COMPOSED OF RX(1), RX(2), RX(26), RX(33), RX(19)  
 RX(137) A + B + BC + J + AJ ==> AQ



AQ  
 YIELD 68%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH  
 SOL 68-12-2 DMF  
 CON 2 hours, room temperature



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STAGE(2)

RCT B 105-39-5  
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
RGT G ~~7803-57-8~~ N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(26) RCT F 41838-25-9, BC 100-52-7

STAGE(1)

CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)

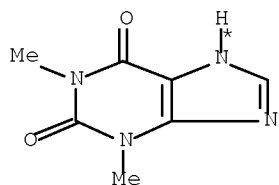
RCT J ~~70-49-5~~  
CAT ~~7646-85-7~~ ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO BD 901781-67-7  
NTE intermediate was isolated

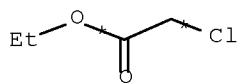
RX(33) RCT BD 901781-67-7  
RGT Q 7719-09-7 SOCl2  
PRO AF 901781-74-6  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(19) RCT AF 901781-74-6, AJ 6066-82-6  
RGT U 121-44-8 Et3N  
PRO AQ ~~901781-60-0~~  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

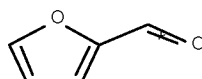
RX(138) OF 139 COMPOSED OF RX(1), RX(2), RX(27), RX(34), RX(12)  
RX(138) A + B + BE + J + S ==> AI



A

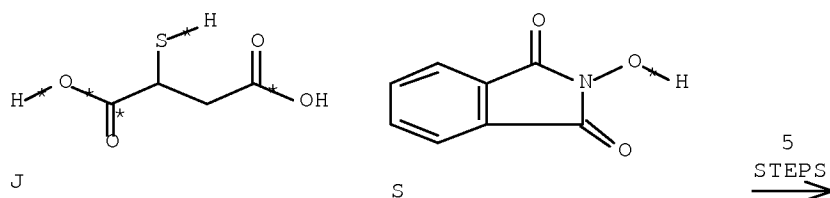


B



BE

10/595943



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5

CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1

RGT G 7803-57-8 N2H4-H2O

PRO F 41838-25-9

SOL 123-91-1 Dioxane

CON 6 hours, reflux

RX(27) RCT F 41838-25-9, BE 98-01-1

STAGE(1)

CAT 64-19-7 AcOH

SOL 64-17-5 EtOH

CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5

CAT 7646-85-7 ZnCl2

SOL 109-99-9 THF

CON 10 hours, reflux

PRO BF 901781-68-8

NTE intermediate was isolated

RX(34) RCT BF 901781-68-8

RGT Q 7719-09-7 SOCl2

PRO AH 901781-75-7

SOL 108-88-3 PhMe

CON 30 minutes, reflux

RX(12) RCT AH 901781-75-7, S 524-38-9

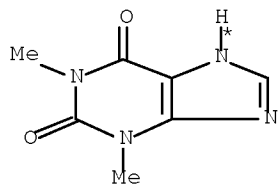
RGT U 121-44-8 Et3N

PRO AI 901781-53-1

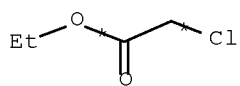
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SOL 68-12-2 DMF  
CON 6 hours, room temperature

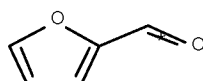
RX(139) OF 139 COMPOSED OF RX(1), RX(2), RX(27), RX(34), RX(20)  
RX(139) A + B + BE + J + AJ ==> AR



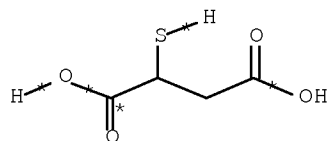
A



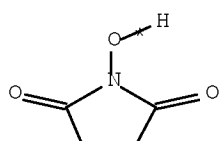
B



BE

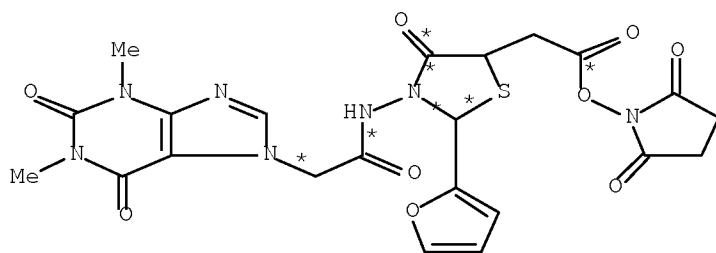


J



AJ

5  
STEPS  
→



AR  
YIELD 58%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5  
CON 6 hours, reflux

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PRO C 7029-96-1

RX(2) RCT C 7029-96-1  
RGT G ~~7803-57-8~~ N2H4-H2O  
PRO F 41838-25-9  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(27) RCT F 41838-25-9, BE 98-01-1

STAGE(1)  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

STAGE(2)  
RCT J ~~70-49-5~~  
CAT ~~7646-85-7~~ ZnCl2  
SOL 109-99-9 THF  
CON 10 hours, reflux

PRO BF 901781-68-8  
NTE intermediate was isolated

RX(34) RCT BF 901781-68-8  
RGT Q 7719-09-7 SOCl2  
PRO AH 901781-75-7  
SOL 108-88-3 PhMe  
CON 30 minutes, reflux

RX(20) RCT AH 901781-75-7, AJ 6066-82-6  
RGT U 121-44-8 Et3N  
PRO AR ~~901781-61-1~~  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

L91 ANSWER 4 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 145:62814 CASREACT Full-text

TITLE: Synthesis and antimicrobial activity of phthalimido  
(2-aryl-3-isonicotinamido-4-oxo-1,3-thiazolidin-5-yl)ethanoates

AUTHOR(S): Sharma, Ranjana; Ahmed, M.; Sharma, Kanika; Talesara,  
G. L.

CORPORATE SOURCE: Department of Botany and Department of Chemistry, M.  
L. Sukhadia University, Udaipur, 313 001, India

SOURCE: Indian Journal of Pharmaceutical Sciences (2005),  
67(4), 462-466  
CODEN: IJSIDW; ISSN: 0250-474X

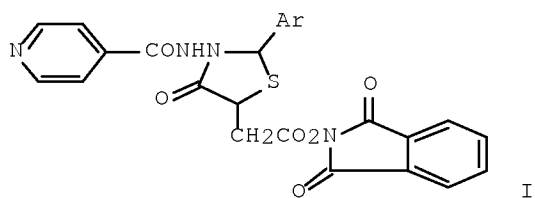
PUBLISHER: Indian Pharmaceutical Association

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

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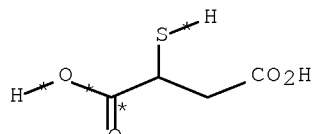
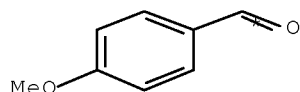
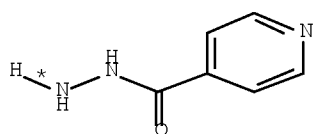


AB Title compds. I [Ar = (un)substituted Ph, 2-furanyl] were prepared in 4 steps starting from isoniazid and ArCHO and including a heterocyclization reaction of mercaptosuccinic acid. All the synthesized compds. were screened for antibacterial (*Bacillus subtilis*, *Escherichia coli*, *Klebsiella pneumoniae*, *Proteus vulgaris*, *Pseudomonas aeruginosa* and *Salmonella typhi*) and antifungal (*Candida albicans* and *Aspergillus fumigatus*) activities. All the compds. exhibited significant activity against the bacteria and fungi tested.

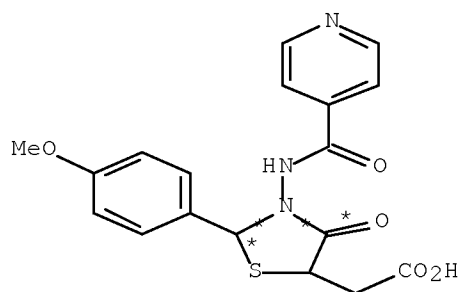
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(33) OF 80 COMPOSED OF RX(1), RX(9)

RX(33) A + B + T ==> U



2  
STEPS  
→



YIELD 78%

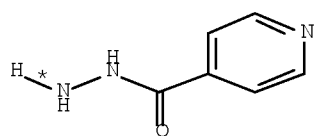
10/595943

RX(1) RCT A 54-85-3, B 123-11-5  
RGT D 64-19-7 AcOH  
PRO C 893-42-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

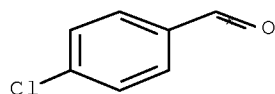
RX(9) RCT C 893-42-5, T 70-49-5  
PRO U 103706-40-7  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 8 hours, reflux

RX(34) OF 80 COMPOSED OF RX(2), RX(10)

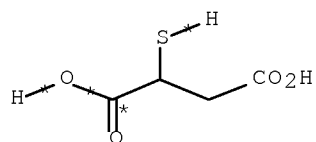
RX(34) A + F + T ==> X



A

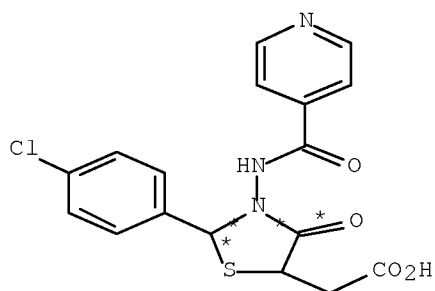


F



T

2  
STEPS  
→



X  
YIELD 71%

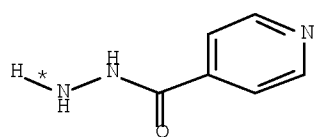
RX(2) RCT A 54-85-3, F 104-88-1  
RGT D 64-19-7 AcOH

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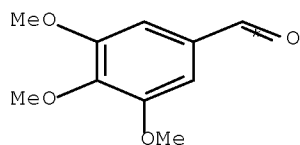
PRO G 6342-46-7  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(10) RCT G 6342-46-7, T 70-49-5  
PRO X 103710-50-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 8 hours, reflux

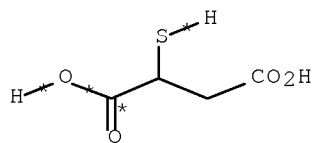
RX(35) OF 80 COMPOSED OF RX(3), RX(11)  
RX(35) A + H + T ==> Y



A

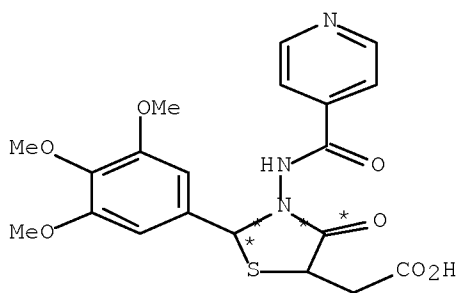


H



T

2  
STEPS  
→



Y  
YIELD 70%

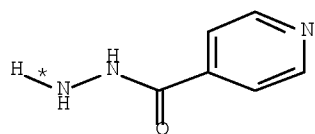
RX(3) RCT A 54-85-3, H 86-81-7  
RGT D 64-19-7 AcOH  
PRO I 67837-40-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(11) RCT I 67837-40-5, T 70-49-5  
PRO Y 890848-58-5

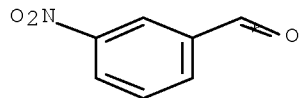
10/595943

CAT 7646-85-7 ZnCl<sub>2</sub>  
 SOL 109-99-9 THF  
 CON 8 hours, reflux

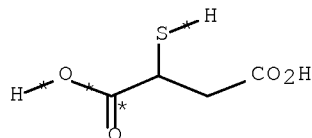
RX(36) OF 80 COMPOSED OF RX(4), RX(12)  
 RX(36) A + J + T ==> Z



A

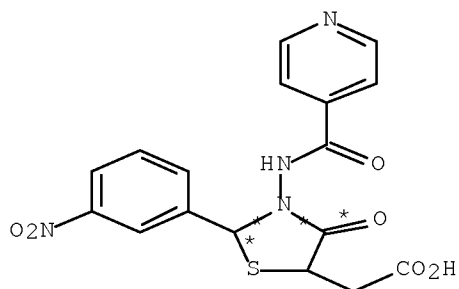


J



T

2  
 STEPS  
 →



Z  
 YIELD 73%

RX(4) RCT A 54-85-3, J 99-61-6  
 RGT D 64-19-7 AcOH  
 PRO K 16012-26-3  
 SOL 64-17-5 EtOH  
 CON 4 hours, reflux

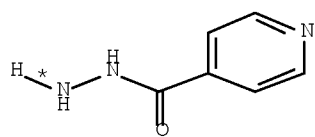
RX(12) RCT K 16012-26-3, T 70-49-5  
 PRO Z 103706-31-6  
 CAT 7646-85-7 ZnCl<sub>2</sub>  
 SOL 109-99-9 THF  
 CON 8 hours, reflux

RX(37) OF 80 COMPOSED OF RX(5), RX(13)

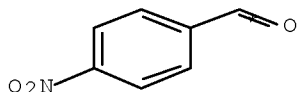


10/595943

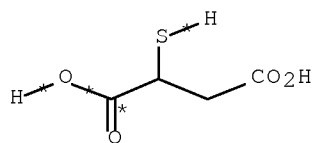
RX(37)      A   +   L   +   T   ==>   AA



A

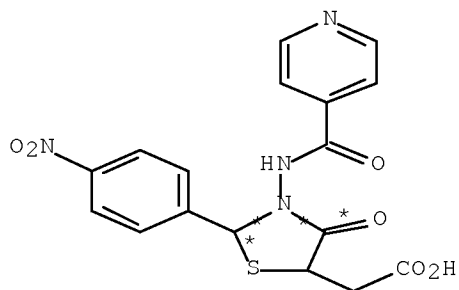


L



T

2  
STEPS  
→



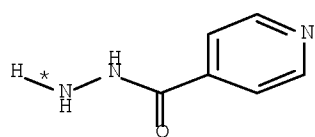
AA  
YIELD 76%

RX(5)      RCT   A 54-85-3, L 555-16-8  
             RGT   D 64-19-7 AcOH  
             PRO   M 4813-07-4  
             SOL   64-17-5 EtOH  
             CON   4 hours, reflux

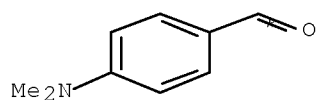
RX(13)     RCT   M 4813-07-4, T 76-49-5  
             PRO   AA 103706-32-7  
             CAT   7646-85-7 ZnCl2  
             SOL   109-99-9 THF  
             CON   8 hours, reflux

RX(38) OF 80 COMPOSED OF RX(6), RX(14)  
RX(38)      A   +   N   +   T   ==>   AB

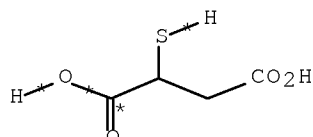
10/595943



A

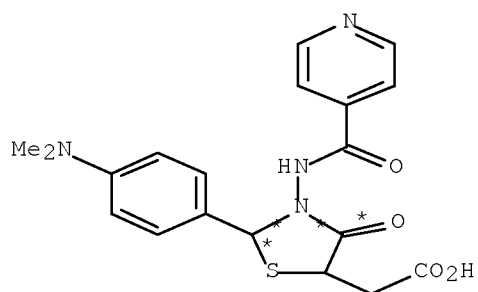


N



T

2  
STEPS  
→



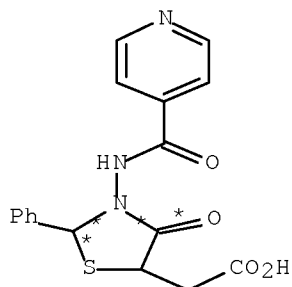
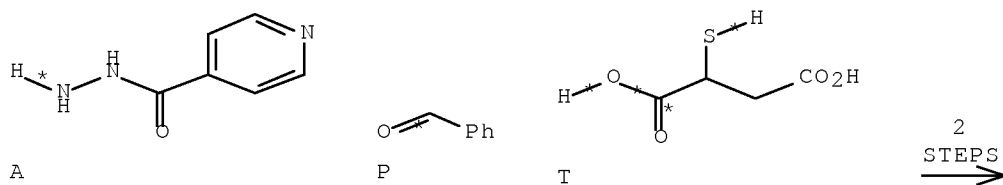
AB  
YIELD 74%

RX(6)      RCT    A 54-85-3, N 100-10-7  
             RGT    D 64-19-7 AcOH  
             PRO    O 13059-77-3  
             SOL    64-17-5 EtOH  
             CON    4 hours, reflux

RX(14)     RCT    O 13059-77-3, T 70-49-5  
             PRO    AB 93607-15-9  
             CAT    7646-85-7 ZnCl2  
             SOL    109-99-9 THF  
             CON    8 hours, reflux

RX(39) OF 80 COMPOSED OF RX(7), RX(15)  
RX(39)      A + P + T ==> AC

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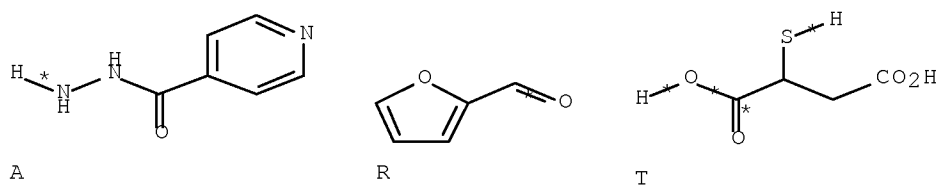


AC  
YIELD 69%

RX(7)        RCT    A 54-85-3, P 100-52-7  
               RGT    D 64-19-7 AcOH  
               PRO    Q 533-02-8  
               SOL    64-17-5 EtOH  
               CON    4 hours, reflux

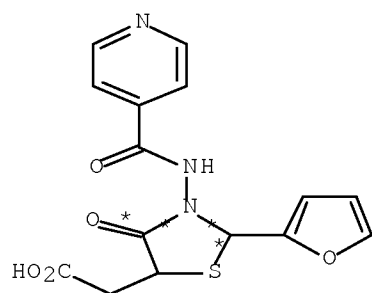
RX(15)      RCT    Q 533-02-8, T 70-49-5  
               PRO    AC 24327-74-0  
               CAT    7646-85-7 ZnCl2  
               SOL    109-99-9 THF  
               CON    8 hours, reflux

RX(40) OF 80 COMPOSED OF RX(8), RX(16)  
 RX(40)        A + R + T ==> AD



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2  
STEPS  
→

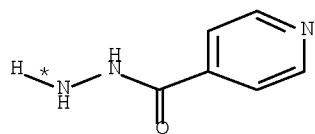


AD  
YIELD 65%

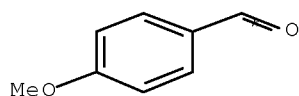
RX(8) RCT A 54-85-3, R 98-01-1  
RGT D 64-19-7 AcOH  
PRO S 6956-53-2  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(16) RCT S 6956-53-2, T 70-49-5  
PRO AD 103706-42-9  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 8 hours, reflux

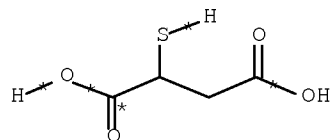
RX(57) OF 80 COMPOSED OF RX(1), RX(9), RX(17)  
RX(57) A + B + T ==> AE



A



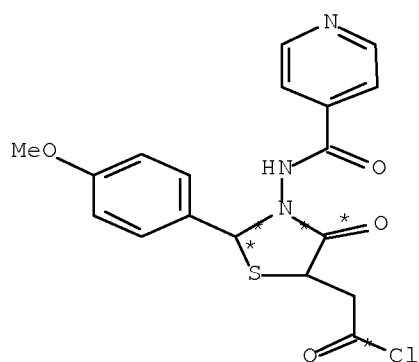
B



T

3  
STEPS  
→

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AE  
YIELD 62%

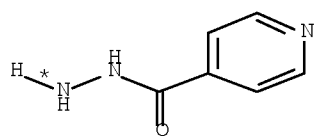
RX(1) RCT A 54-85-3, B 123-11-5  
RGT D 64-19-7 AcOH  
PRO C 893-42-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(9) RCT C 893-42-5, T 70-49-5  
PRO U 103706-40-7  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 8 hours, reflux

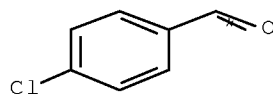
RX(17) RCT U 103706-40-7  
RGT AF 7719-09-7 SOCl2  
PRO AE 890848-59-6  
SOL 71-43-2 Benzene  
CON 60 minutes, reflux

RX(58) OF 80 COMPOSED OF RX(2), RX(10), RX(18)

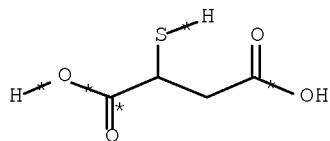
RX(58) A + F + T ==> AE



A



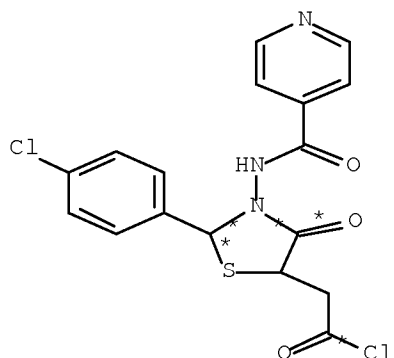
F



T

3  
STEPS  
→

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AH  
YIELD 60%

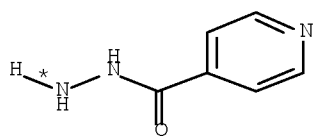
RX(2) RCT A 54-85-3, F 104-88-1  
RGT D 64-19-7 AcOH  
PRO G 6342-46-7  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(10) RCT G 6342-46-7, T 70-49-5  
PRO X 103710-50-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 8 hours, reflux

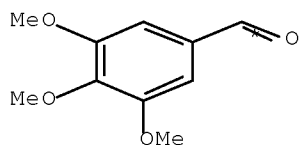
RX(18) RCT X 103710-50-5  
RGT AF 7719-09-7 SOCl2  
PRO AH 890848-60-9  
SOL 71-43-2 Benzene  
CON 60 minutes, reflux

RX(59) OF 80 COMPOSED OF RX(3), RX(11), RX(19)

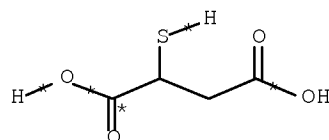
RX(59) A + H + T ==> AI



A



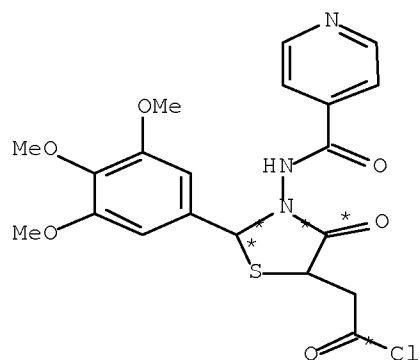
H



T

10/595943

3  
STEPS  
→



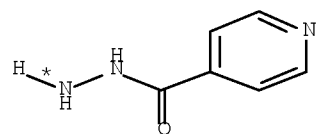
AI  
YIELD 66%

RX(3) RCT A 54-85-3, H 86-81-7  
RGT D 64-19-7 AcOH  
PRO I 67837-40-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

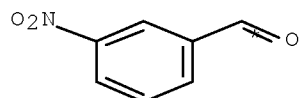
RX(11) RCT I 67837-40-5, T 70-49-5  
PRO Y 890848-58-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 8 hours, reflux

RX(19) RCT Y 890848-58-5  
RGT AF 7719-09-7 SOCl2  
PRO AI 890848-61-0  
SOL 71-43-2 Benzene  
CON 60 minutes, reflux

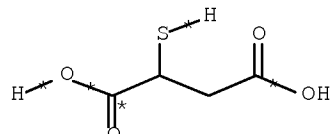
RX(60) OF 80 COMPOSED OF RX(4), RX(12), RX(20)  
RX(60) A + J + T ==> AJ



A



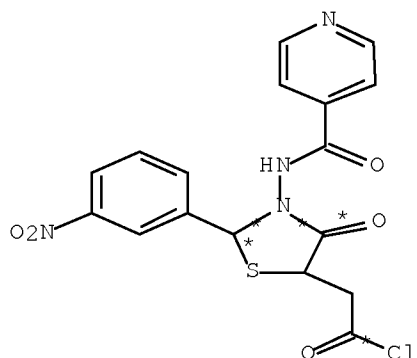
J



T

10/595943

3  
STEPS  
→



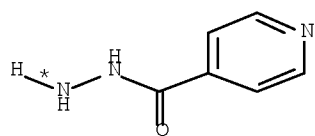
AJ  
YIELD 58%

RX(4) RCT A 54-85-3, J 99-61-6  
RGT D 64-19-7 AcOH  
PRO K 16012-26-3  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

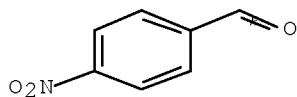
RX(12) RCT K 16012-26-3, T 70-49-5  
PRO Z 103706-31-6  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 8 hours, reflux

RX(20) RCT Z 103706-31-6  
RGT AF 7719-09-7 SOCl2  
PRO AJ 890848-62-1  
SOL 71-43-2 Benzene  
CON 60 minutes, reflux

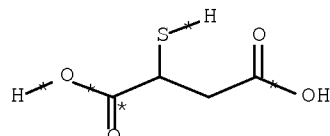
RX(61) OF 80 COMPOSED OF RX(5), RX(13), RX(21)  
RX(61) A + L + T ==> AK



A



L

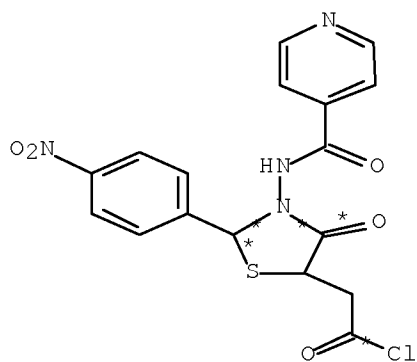


T



10/595943

3  
STEPS  
→



AK  
YIELD 55%

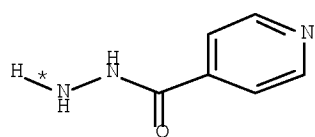
RX(5)      RCT    A 54-85-3, L 555-16-8  
             RGT    D 64-19-7 AcOH  
             PRO    M 4813-07-4  
             SOL    64-17-5 EtOH  
             CON    4 hours, reflux

RX(13)     RCT    M 4813-07-4, T 70-49-5  
             PRO    AA 103706-32-7  
             CAT    7646-85-7 ZnCl2  
             SOL    109-99-9 THF  
             CON    8 hours, reflux

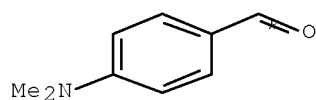
RX(21)     RCT    AA 103706-32-7  
             RGT    AF 7719-09-7 SOCl2  
             PRO    AK 890848-63-2  
             SOL    71-43-2 Benzene  
             CON    60 minutes, reflux

RX(62) OF 80 COMPOSED OF RX(6), RX(14), RX(22)  
RX(62)      A   +   N   +   T   ==>   AL

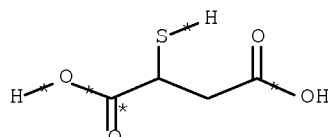
10/595943



A

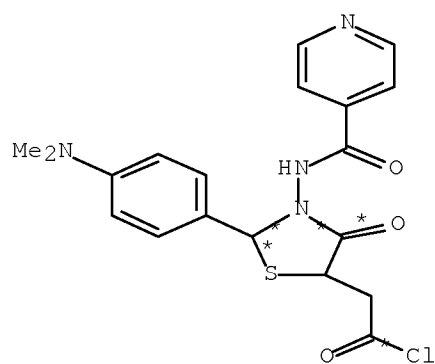


N



T

3  
STEPS  
→



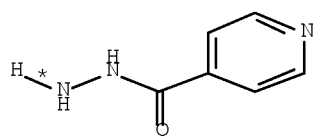
AL  
YIELD 67%

RX(6)	RCT	A 54-85-3, N 100-10-7
	RGT	D 64-19-7 AcOH
	PRO	O 13059-77-3
	SOL	64-17-5 EtOH
	CON	4 hours, reflux
RX(14)	RCT	O 13059-77-3, T 70-49-5
	PRO	AB 93607-15-9
	CAT	7646-85-7 ZnCl2
	SOL	109-99-9 THF
	CON	8 hours, reflux
RX(22)	RCT	AB 93607-15-9
	RGT	AF 7719-09-7 SOCl2
	PRO	AL 890848-64-3
	SOL	71-43-2 Benzene
	CON	60 minutes, reflux

RX(63) OF 80 COMPOSED OF RX(7), RX(15), RX(23)

10/595943

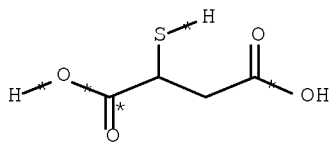
RX(63)      A   +   P   +   T   ==>   AM



A

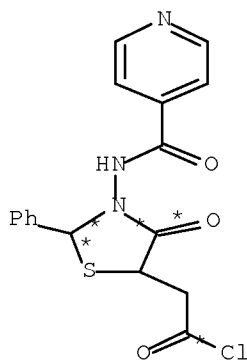


P



T

3  
STEPS  
→



AM  
YIELD 53%

RX(7)      RCT    A 54-85-3, P 100-52-7  
             RGT    D 64-19-7 AcOH  
             PRO    Q 533-02-8  
             SOL    64-17-5 EtOH  
             CON    4 hours, reflux

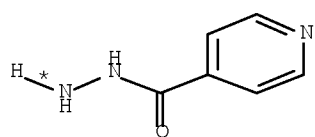
RX(15)     RCT    Q 533-02-8, T 70-49-5  
             PRO    AC 24327-74-0  
             CAT    7646-85-7 ZnCl2  
             SOL    109-99-9 THF  
             CON    8 hours, reflux

RX(23)     RCT    AC 24327-74-0  
             RGT    AF 7719-09-7 SOCl2  
             PRO    AM 890848-65-4  
             SOL    71-43-2 Benzene  
             CON    60 minutes, reflux

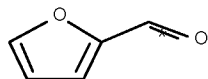
RX(64) OF 80 COMPOSED OF RX(8), RX(16), RX(24)

RX(64)      A   +   R   +   T   ==>   AN

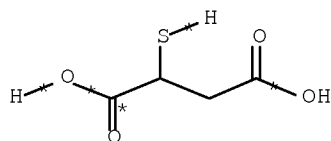
10/595943



A

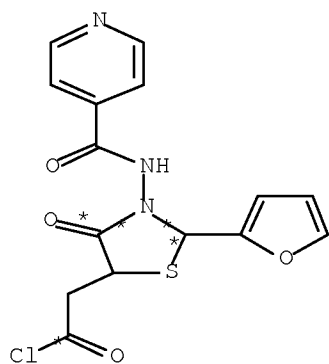


R



T

3  
STEPS  
→



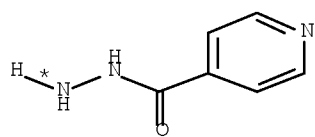
AN  
YIELD 59%

RX(8)	RCT	A 54-85-3, R 98-01-1
	RGT	D 64-19-7 AcOH
	PRO	S 6956-53-2
	SOL	64-17-5 EtOH
	CON	4 hours, reflux
RX(16)	RCT	S 6956-53-2, T 70-49-5
	PRO	AD 103706-42-9
	CAT	7646-85-7 ZnCl <sub>2</sub>
	SOL	109-99-9 THF
	CON	8 hours, reflux
RX(24)	RCT	AD 103706-42-9
	RGT	AF 7719-09-7 SOCl <sub>2</sub>
	PRO	AN 890848-66-5
	SOL	71-43-2 Benzene
	CON	60 minutes, reflux

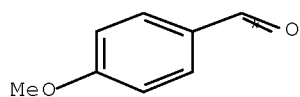
RX(66) OF 80 COMPOSED OF RX(1), RX(9), RX(17), RX(25)

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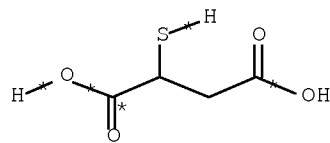
RX(66)      A + B + T + AO ==> AP



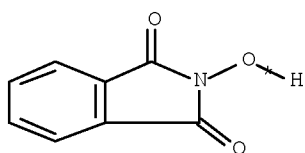
A



B

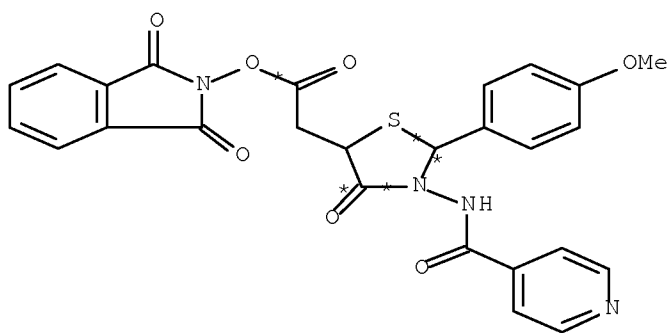


T



AO

4  
STEPS  
→



AP  
YIELD 73%

RX(1)      RCT    A 54-85-3, B 123-11-5  
              RGT    D 64-19-7 AcOH  
              PRO    C 893-42-5  
              SOL    64-17-5 EtOH  
              CON    4 hours, reflux

RX(9)      RCT    C 893-42-5, T 70-49-5  
              PRO    U 103706-40-7  
              CAT    7646-85-7 ZnCl2  
              SOL    109-99-9 THF  
              CON    8 hours, reflux

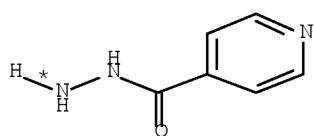
RX(17)     RCT    U 103706-40-7

10/595943

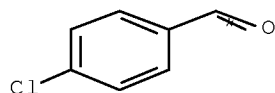
RGT AF 7719-09-7 SOC12  
PRO AE 890848-59-6  
SOL 71-43-2 Benzene  
CON 60 minutes, reflux

RX(25) RCT AE 890848-59-6, AO 524-38-9  
RGT AQ 121-44-8 Et3N  
PRO AP 890848-67-6  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 1 hour, room temperature  
SUBSTAGE(2) room temperature -> reflux  
SUBSTAGE(3) 3 hours, reflux

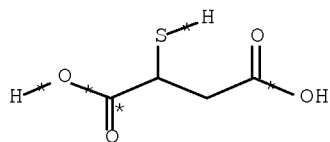
RX(68) OF 80 COMPOSED OF RX(2), RX(10), RX(18), RX(26)  
RX(68) A + F + T + AO ==> AS



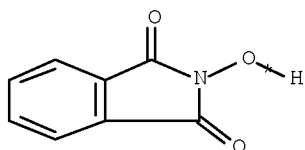
A



F

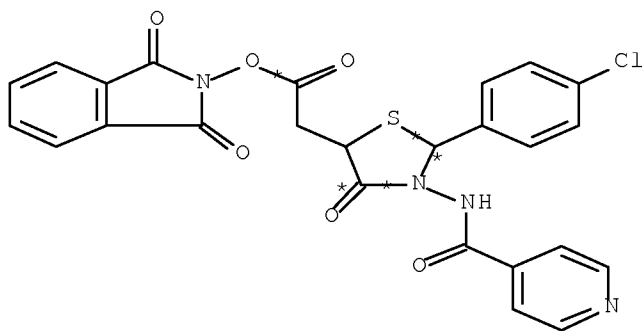


T



AO

4  
STEPS  
→



AS  
YIELD 68%

10/595943

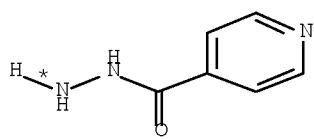
RX(2) RCT A 54-85-3, F 104-88-1  
 RGT D 64-19-7 AcOH  
 PRO G 6342-46-7  
 SOL 64-17-5 EtOH  
 CON 4 hours, reflux

RX(10) RCT G 6342-46-7, T 70-49-5  
 PRO X 103710-50-5  
 CAT 7646-85-7 ZnCl2  
 SOL 109-99-9 THF  
 CON 8 hours, reflux

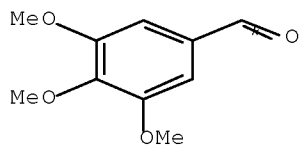
RX(18) RCT X 103710-50-5  
 RGT AF 7719-09-7 SOCl2  
 PRO AH 890848-60-9  
 SOL 71-43-2 Benzene  
 CON 60 minutes, reflux

RX(26) RCT AH 890848-60-9, AO 524-38-9  
 RGT AQ 121-44-8 Et3N  
 PRO AS 890848-68-7  
 SOL 68-12-2 DMF  
 CON SUBSTAGE(1) 1 hour, room temperature  
 SUBSTAGE(2) room temperature -> reflux  
 SUBSTAGE(3) 3 hours, reflux

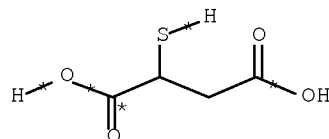
RX(70) OF 80 COMPOSED OF RX(3), RX(11), RX(19), RX(27)  
 RX(70) A + H + T + AO ==> AT



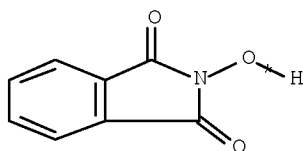
A



H



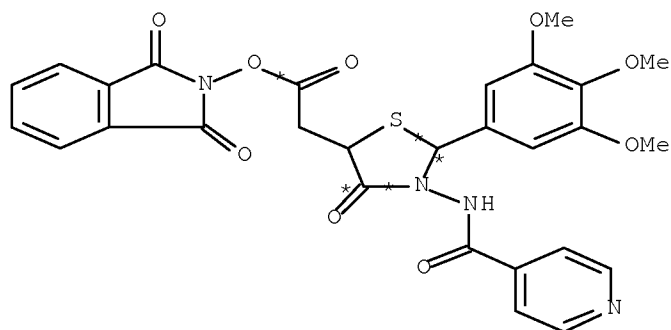
T



AO

4  
STEPS  
→

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AT  
YIELD 70%

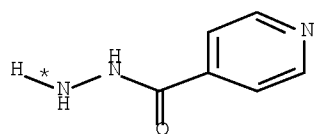
RX(3) RCT A 54-85-3, H 86-81-7  
RGT D 64-19-7 AcOH  
PRO I 67837-40-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(11) RCT I 67837-40-5, T 70-49-5  
PRO Y 890848-58-5  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 8 hours, reflux

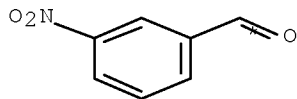
RX(19) RCT Y 890848-58-5  
RGT AF 7719-09-7 SOCl2  
PRO AI 890848-61-0  
SOL 71-43-2 Benzene  
CON 60 minutes, reflux

RX(27) RCT AI 890848-61-0, AO 524-38-9  
RGT AQ 121-44-8 Et3N  
PRO AT 890848-69-8  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 1 hour, room temperature  
SUBSTAGE(2) room temperature -> reflux  
SUBSTAGE(3) 3 hours, reflux

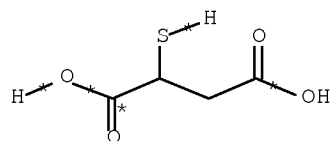
RX(72) OF 80 COMPOSED OF RX(4), RX(12), RX(20), RX(28)  
RX(72) A + J + T + AO ==> AU



A



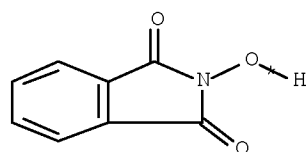
J



T

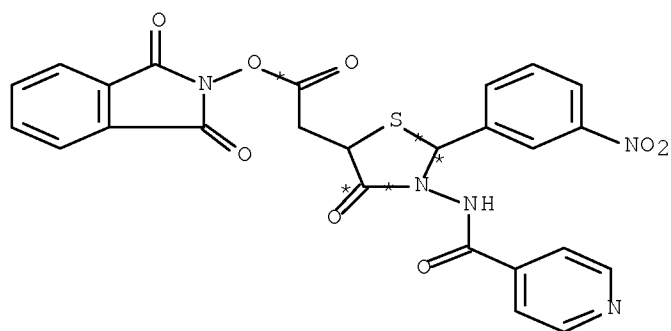


10/595943



AO

4  
STEPS  
→



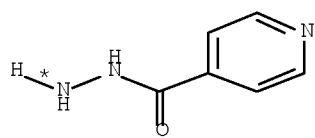
AU  
YIELD 63%

RX(4)	RCT	A 54-85-3, J 99-61-6
	RGT	D 64-19-7 AcOH
	PRO	K 16012-26-3
	SOL	64-17-5 EtOH
	CON	4 hours, reflux
RX(12)	RCT	K 16012-26-3, T 70-49-5
	PRO	Z 103706-31-6
	CAT	7646-85-7 ZnCl2
	SOL	109-99-9 THF
	CON	8 hours, reflux
RX(20)	RCT	Z 103706-31-6
	RGT	AF 7719-09-7 SOCl2
	PRO	AJ 890848-62-1
	SOL	71-43-2 Benzene
	CON	60 minutes, reflux
RX(28)	RCT	AJ 890848-62-1, AO 524-38-9
	RGT	AQ 121-44-8 Et3N
	PRO	AU 890848-70-1
	SOL	68-12-2 DMF
	CON	SUBSTAGE(1) 1 hour, room temperature
		SUBSTAGE(2) room temperature -> reflux
		SUBSTAGE(3) 3 hours, reflux

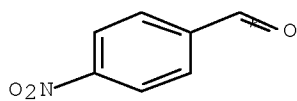
10/595943

RX(74) OF 80 COMPOSED OF RX(5), RX(13), RX(21), RX(29)

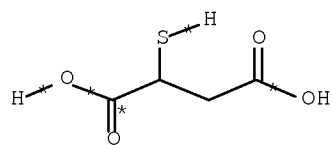
RX(74) A + L + T + AO ==> AV



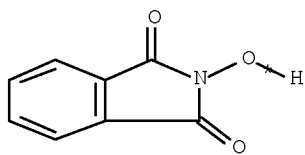
A



L

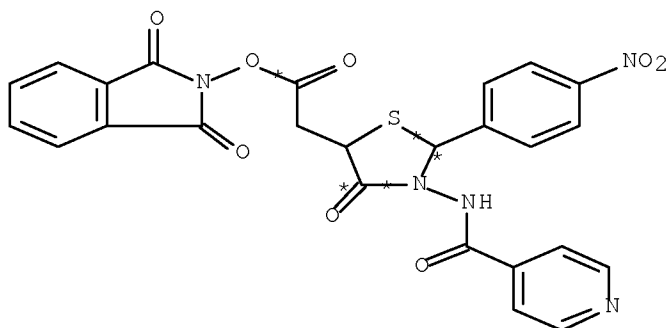


T



AO

4  
STEPS  
→



AV  
YIELD 60%

RX(5) RCT A 54-85-3, L 555-16-8  
RGT D 64-19-7 AcOH  
PRO M 4813-07-4  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(13) RCT M 4813-07-4, T 70-49-5  
PRO AA 103706-32-7  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 8 hours, reflux

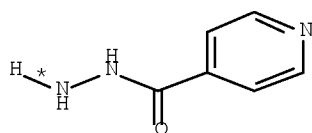
10/595943

RX(21) RCT AA 103706-32-7  
 RGT AF 7719-09-7 SOC12  
 PRO AK 890848-63-2  
 SOL 71-43-2 Benzene  
 CON 60 minutes, reflux

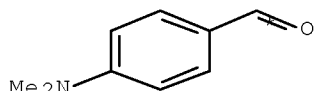
RX(29) RCT AK 890848-63-2, AO 524-38-9  
 RGT AQ 121-44-8 Et3N  
 PRO AV 890848-71-2  
 SOL 68-12-2 DMF  
 CON SUBSTAGE(1) 1 hour, room temperature  
 SUBSTAGE(2) room temperature -> reflux  
 SUBSTAGE(3) 3 hours, reflux

RX(76) OF 80 COMPOSED OF RX(6), RX(14), RX(22), RX(30)

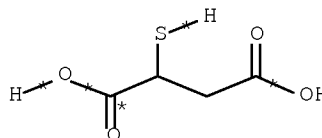
RX(76) A + N + T + AO ==> AW



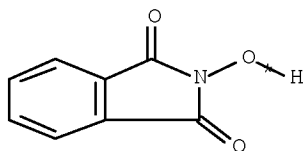
A



N

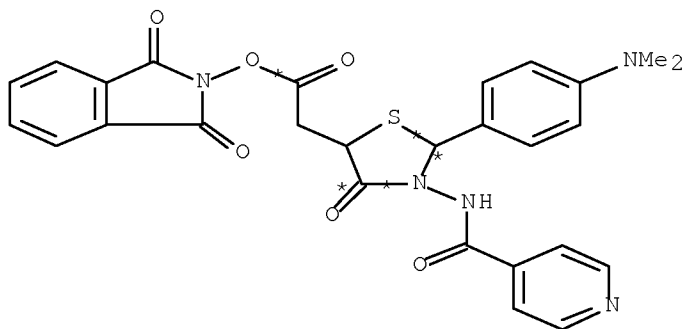


T



AO

4  
STEPS  
→



AW  
YIELD 59%

10/595943

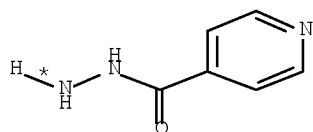
RX(6) RCT A 54-85-3, N 100-10-7  
 RGT D 64-19-7 AcOH  
 PRO O 13059-77-3  
 SOL 64-17-5 EtOH  
 CON 4 hours, reflux

RX(14) RCT O 13059-77-3, T 70-49-5  
 PRO AB 93607-15-9  
 CAT 7646-85-7 ZnCl2  
 SOL 109-99-9 THF  
 CON 8 hours, reflux

RX(22) RCT AB 93607-15-9  
 RGT AF 7719-09-7 SOCl2  
 PRO AL 890848-64-3  
 SOL 71-43-2 Benzene  
 CON 60 minutes, reflux

RX(30) RCT AL 890848-64-3, AO 524-38-9  
 RGT AQ 121-44-8 Et3N  
 PRO AW 890848-72-3  
 SOL 68-12-2 DMF  
 CON SUBSTAGE(1) 1 hour, room temperature  
 SUBSTAGE(2) room temperature -> reflux  
 SUBSTAGE(3) 3 hours, reflux

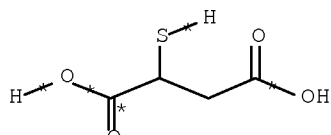
RX(78) OF 80 COMPOSED OF RX(7), RX(15), RX(23), RX(31)  
 RX(78) A + P + T + AO ==> AX



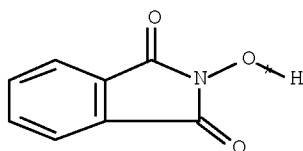
A



P



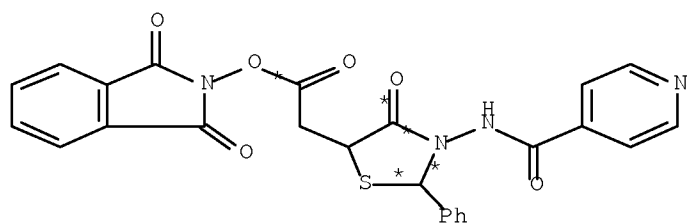
T



AO

4  
STEPS  
→

10/595943



AX  
YIELD 65%

RX(7) RCT A 54-85-3, P 100-52-7  
RGT D 64-19-7 AcOH  
PRO Q 533-02-8  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

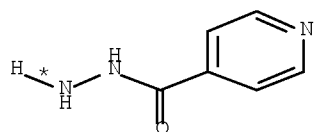
RX(15) RCT Q 533-02-8, T 70-49-5  
PRO AC 24327-74-0  
CAT 7646-85-7 ZnCl2  
SOL 109-99-9 THF  
CON 8 hours, reflux

RX(23) RCT AC 24327-74-0  
RGT AF 7719-09-7 SOCl2  
PRO AM 890848-65-4  
SOL 71-43-2 Benzene  
CON 60 minutes, reflux

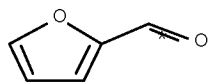
RX(31) RCT AM 890848-65-4, AO 524-38-9  
RGT AQ 121-44-8 Et3N  
PRO AX 890848-73-4  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 1 hour, room temperature  
SUBSTAGE(2) room temperature -> reflux  
SUBSTAGE(3) 3 hours, reflux

RX(80) OF 80 COMPOSED OF RX(8), RX(16), RX(24), RX(32)

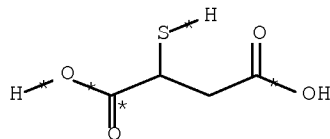
RX(80) A + R + T + AO ==> AY



A

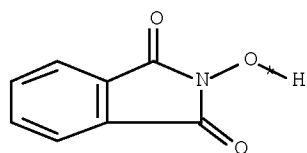


R



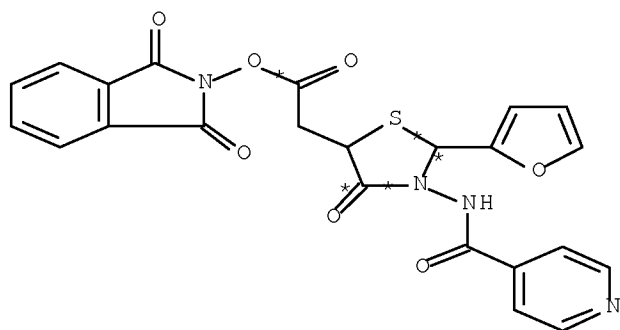
T

10/595943



AO

4  
STEPS  
→



AY  
YIELD 74%

RX(8)	RCT	A 54-85-3, R 98-01-1
	RGT	D 64-19-7 AcOH
	PRO	S 6956-53-2
	SOL	64-17-5 EtOH
	CON	4 hours, reflux
RX(16)	RCT	S 6956-53-2, T 70-49-5
	PRO	AD 103706-42-9
	CAT	7646-85-7 ZnCl <sub>2</sub>
	SOL	109-99-9 THF
	CON	8 hours, reflux
RX(24)	RCT	AD 103706-42-9
	RGT	AF 7719-09-7 SOCl <sub>2</sub>
	PRO	AN 890848-66-5
	SOL	71-43-2 Benzene
	CON	60 minutes, reflux
RX(32)	RCT	AN 890848-66-5, AO 524-38-9
	RGT	AQ 121-44-8 Et <sub>3</sub> N
	PRO	AY 890848-74-5
	SOL	68-12-2 DMF
	CON	SUBSTAGE(1) 1 hour, room temperature
		SUBSTAGE(2) room temperature -> reflux
		SUBSTAGE(3) 3 hours, reflux

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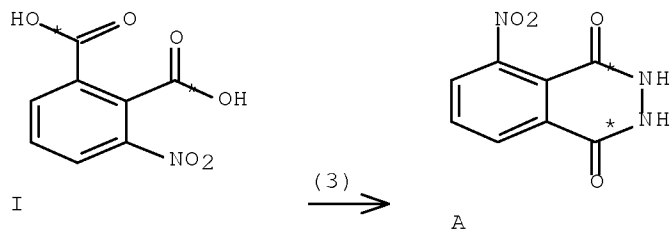
ACCESSION NUMBER: 143:26622 CASREACT Full-text  
 TITLE: Hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids  
 INVENTOR(S): Lopes, Claudio Cerqueira; Lopes, Rosangela Sabattini Capella; Cardoso, Jari Nobrega; Alves Da Silva, Jacqueline; Ferreira Gomes, Leticia  
 PATENT ASSIGNEE(S): Universidade Federal do Rio de Janeiro-UFRJ, Brazil  
 SOURCE: PCT Int. Appl., 14 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005051870	A2	20050609	WO 2004-BR236	20041125
WO 2005051870	A3	20050707		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
BR 2003007864	A	20050705	BR 2003-7864	20031125
US 20070128680	A1	20070607	US 2006-595943	20060522
PRIORITY APPLN. INFO.:			BR 2003-7864	20031125
			WO 2004-BR236	20041125

OTHER SOURCE(S): MARPAT 143:26622

AB A process to form hydrazides (e.g., luminol) from the reaction of a hydrazine and a dicarboxylic (e.g., 3-nitrophthalic acid) using a Lewis acid catalyst (e.g., niobium pentachloride) is described. The reaction occurs in a safe reactional environment, utilizing smooth conditions, neither involving high temps. nor high pressures, producing the desired products with high yields, between 90-95%. The invention also describes a kit for utilization of chemiluminescent substances, comprised of two solns.

RX(3) OF 6 ...I ==> A...



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RX(3) RCT I 603-11-2

STAGE(1)

CAT 10026-12-7 NbCl5

CON 30 minutes, room temperature

STAGE(2)

RGT L 302-01-2 N2H4

SOL 7732-18-5 Water

CON SUBSTAGE(1) 30 minutes, room temperature -> 50 deg C

SUBSTAGE(2) 4 hours, 50 deg C

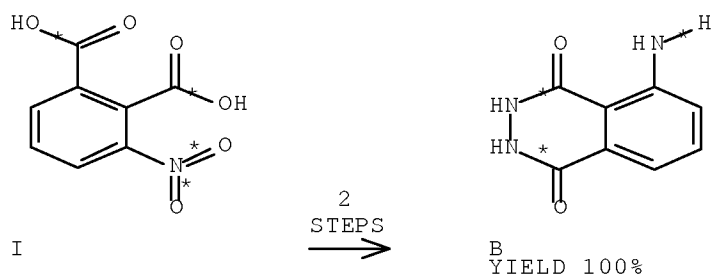
SUBSTAGE(3) cooled

PRO A 3682-15-3

NTE inert

RX(5) OF 6 COMPOSED OF RX(3), RX(1)

RX(5) I ==> B



RX(3) RCT I 603-11-2

STAGE(1)

CAT 10026-12-7 NbCl5

CON 30 minutes, room temperature

STAGE(2)

RGT L 302-01-2 N2H4

SOL 7732-18-5 Water

CON SUBSTAGE(1) 30 minutes, room temperature -> 50 deg C

SUBSTAGE(2) 4 hours, 50 deg C

SUBSTAGE(3) cooled

PRO A 3682-15-3

NTE inert

RX(1) RCT A 3682-15-3

RGT C 1333-74-0 H2

PRO B 521-31-3

CAT 7440-05-3 Pd

SOL 123-91-1 Dioxane, 7732-18-5 Water, 64-19-7 AcOH

CON room temperature

NTE Pd supported on carbon was used as catalyst, sodium dithionite in acidic medium can also be used as reducing agent

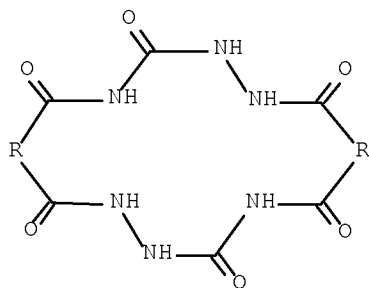


- II Hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids
- AB A process to form hydrazides (e.g., luminol) from the reaction of a hydrazine and a dicarboxylic (e.g., 3-nitrophthalic acid) using a Lewis acid catalyst (e.g., niobium pentachloride) is described. The reaction occurs in a safe reactional environment, utilizing smooth conditions, neither involving high temps. nor high pressures, producing the desired products with high yields, between 90-95%. The invention also describes a kit for utilization of chemiluminescent substances, comprised of two solns.
- IT Amidation  
Amidation catalysts  
(hydrazidation; hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids)
- IT Hydrazides  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids)
- IT Nitration  
Reduction  
(hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids using)
- IT Lewis acids  
RL: CAT (Catalyst use); USES (Uses)  
(hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids using)
- IT 7446-70-0, Aluminum chloride, uses 7447-39-4, Cupric chloride, uses 7487-94-7, MercuryII chloride, uses 7550-45-0, Titanium tetrachloride, uses 7637-07-2, Boron trifluoride, uses 7646-79-9, Cobalt chloride (CoCl<sub>2</sub>), uses 7646-85-7, Zinc chloride, uses 7647-18-9, Antimony pentachloride 7705-07-9, Titanium trichloride, uses 7705-08-0, Ferric chloride, uses 7718-54-9, Nickel chloride, uses 7758-89-6, Cuprous chloride 7784-34-1, Arsenic trichloride 7786-30-3, Magnesium chloride, uses 7787-47-5, Beryllium chloride 7787-60-2, Bismuth trichloride 7789-48-2, Magnesium bromide 10025-73-7, Chromium trichloride 10025-91-9, Antimony trichloride 10026-07-0, Tellurium tetrachloride 10026-10-5, Uranium tetrachloride 10026-11-6, Zirconium tetrachloride 10026-12-7, Niobium pentachloride 10049-06-6, Titanium dichloride 10108-64-2, Cadmium chloride 10294-34-5, Boron trichloride 13450-90-3, Gallium chloride 22441-45-8, Arsenic pentachloride  
RL: CAT (Catalyst use); USES (Uses)  
(hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids)
- IT 7697-37-2, Nitric acid, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids)
- IT 85-44-9, Phthalic anhydride  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids using)
- IT 603-11-2P, 3-Nitrophthalic acid 3682-15-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids using)
- IT 521-31-3P, Luminol  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids using)
- IT 67-64-1, Acetone, uses 67-68-5, DmsO, uses 68-12-2, Dmf, uses

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123-91-1, Dioxane, uses 872-50-4, NMP, uses  
RL: NUU (Other use, unclassified); USES (Uses)  
(solvent; hydrazide catalytic production process from hydrazines and  
dicarboxylic acids in the presence of Lewis acids  
using)

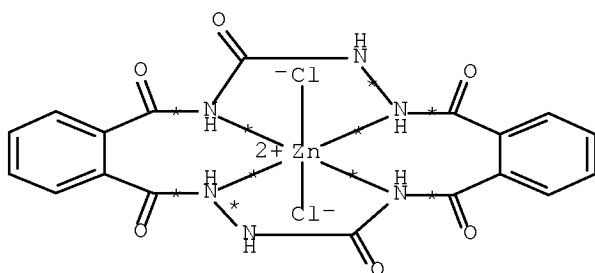
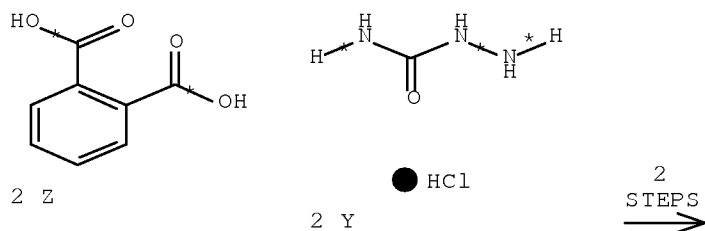
L91 ANSWER 6 OF 30 CASREACT COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 142:474748 CASREACT Full-text  
TITLE: Novel 16-membered [N6] macrocycles bearing hexaamide  
functions and their metal-encapsulated compounds  
AUTHOR(S): Siddiqi, Zafar Ahmad; Shadab, Shah Mohammad  
CORPORATE SOURCE: Division of Inorganic Chemistry, Chemistry Department,  
Aligarh Muslim University, Aligarh, 202002, India  
SOURCE: Indian Journal of Chemistry, Section A: Inorganic,  
Bio-inorganic, Physical, Theoretical & Analytical  
Chemistry (2004), 43A(11), 2274-2280  
CODEN: ICACEC; ISSN: 0376-4710  
PUBLISHER: National Institute of Science Communication  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Cyclocondensation reaction between phthalic anhydride/phthalic acid or succinic anhydride/succinic acid and semicarbazide hydrochloride in DMF-MeOH under reflux affords I.xHCl (R = o-C6H4, x = 0; R = CH2CH2, x = 2). Reactions of the macrocycles with [ML]Cl2 or [M(PPh3)2Cl2] (M = Zn, Cd or Hg) gave MLC12 (L = I). Physicochem. and spectroscopic studies of complexes reveal that proton at aza group (NH) of the amide/peptide function does not deprotonate prior to coordination and hexacoordination around metal ions is maintained.  
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(23) OF 40 COMPOSED OF RX(14), RX(1)  
RX(23) 2 Z + 2 Y ==> B

10/595943

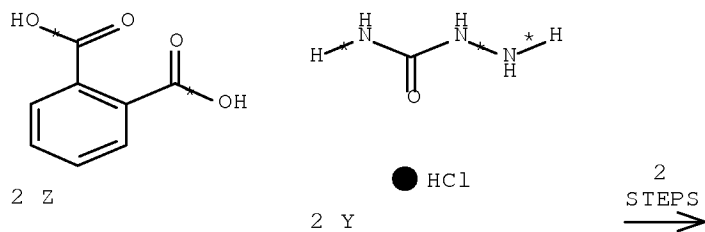


B  
YIELD 23%

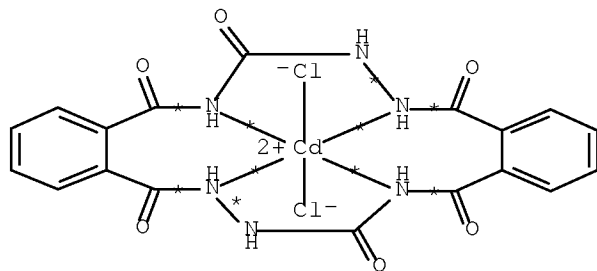
RX(14)      RCT    Z 88-99-3, Y 563-41-7  
              PRO    A 851625-90-6  
              SOL    67-56-1 MeOH, 68-12-2 DMF  
              CON    6 hours, reflux

RX(1)      RCT    A 851625-90-6  
              RGT    C 7646-85-7 ZnCl2  
              PRO    B 851625-78-0  
              SOL    67-56-1 MeOH, 68-12-2 DMF  
              CON    24 hours, room temperature

RX(25) OF 40 COMPOSED OF RX(14), RX(5)  
 RX(25)      2 Z    +    2 Y    ==>    L



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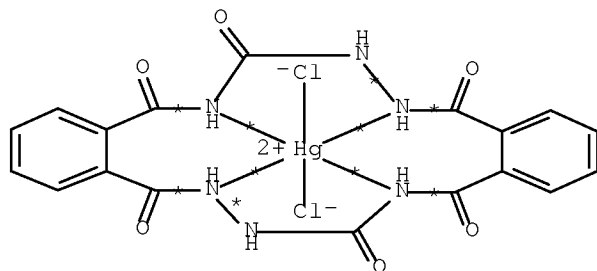
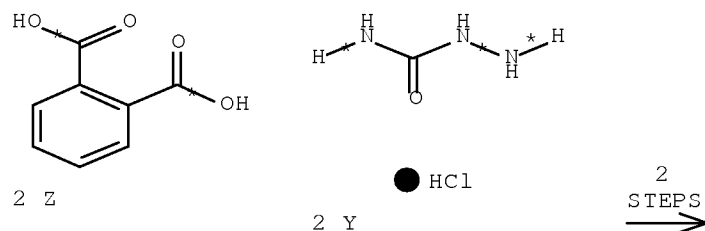
L  
YIELD 42%

RX(14) RCT Z 88-99-3, Y 563-41-7  
PRO A 851625-90-6  
SOL 67-56-1 MeOH, 68-12-2 DMF  
CON 6 hours, reflux

RX(5) RCT A 851625-90-6  
RGT M 10108-64-2 CdCl2  
PRO L 851625-82-6  
SOL 67-56-1 MeOH, 68-12-2 DMF  
CON 24 hours, room temperature

RX(27) OF 40 COMPOSED OF RX(14), RX(9)

RX(27) 2 Z + 2 Y ==> R



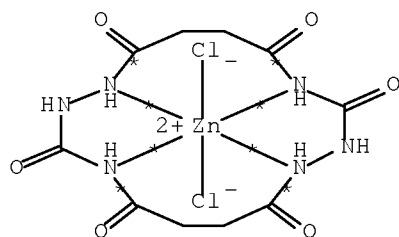
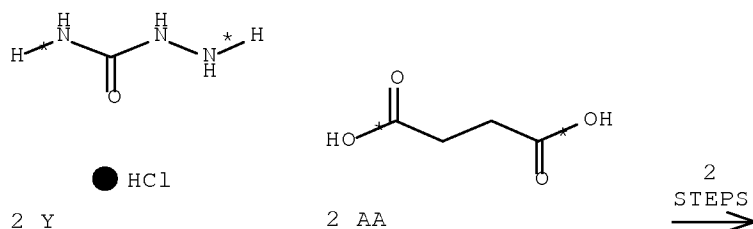
R  
YIELD 36%

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RX(14)      RCT    Z 88-99-3, Y 563-41-7  
             PRO    A 851625-90-6  
             SOL    67-56-1 MeOH, 68-12-2 DMF  
             CON    6 hours, reflux

RX(9)        RCT    A 851625-90-6  
             RGT    S 7487-94-7 HgCl2  
             PRO    R 851625-86-0  
             SOL    67-56-1 MeOH, 68-12-2 DMF  
             CON    24 hours, room temperature

RX(29) OF 40 COMPOSED OF RX(15), RX(3)  
RX(29)       2 Y   +   2 AA   ==>   J



J  
YIELD 22%

RX(15)      RCT    Y 563-41-7

STAGE(1)

RGT    AB 7647-01-0 HCl  
SOL    7732-18-5 Water  
CON    1 hour, room temperature

STAGE(2)

RCT    AA 110-15-6  
SOL    123-91-1 Dioxane  
CON    SUBSTAGE(1) 6 hours, reflux

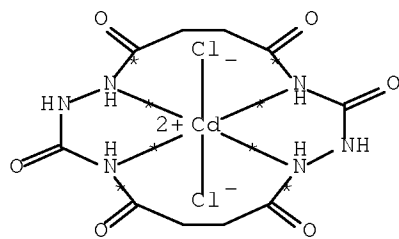
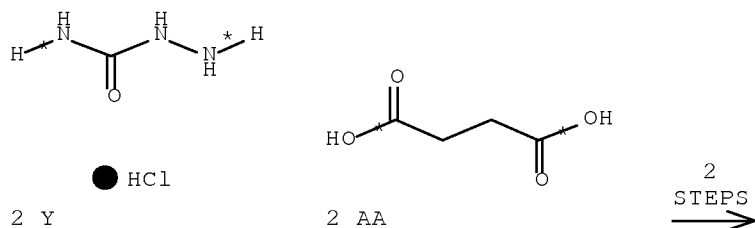
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SUBSTAGE(2) overnight, room temperature

PRO I 851625-91-7

RX(3) RCT I 851625-91-7  
RGT C 7646-85-7 ZnCl2  
PRO J 851625-80-4  
SOL 67-56-1 MeOH, 68-12-2 DMF  
CON 24 hours, room temperature

RX(31) OF 40 COMPOSED OF RX(15), RX(7)  
RX(31) 2 Y + 2 AA ==> P



P  
YIELD 92%

RX(15) RCT Y 563-41-7

STAGE(1)

RGT AB 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON 1 hour, room temperature

STAGE(2)

RCT AA 110-15-6  
SOL 123-91-1 Dioxane  
CON SUBSTAGE(1) 6 hours, reflux  
SUBSTAGE(2) overnight, room temperature

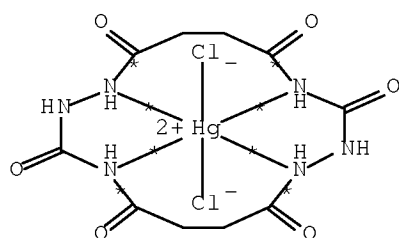
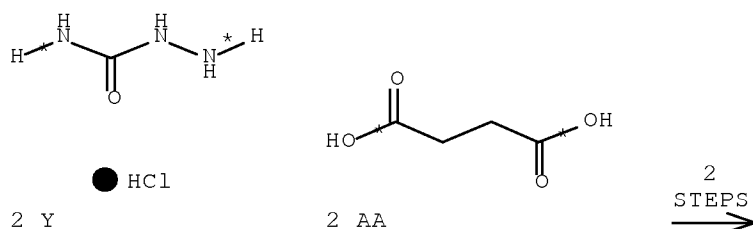
PRO I 851625-91-7

RX(7) RCT I 851625-91-7

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RGT M 10108-64-2 CdCl2  
PRO P 851625-84-8  
SOL 67-56-1 MeOH, 68-12-2 DMF  
CON 24 hours, room temperature

RX(33) OF 40 COMPOSED OF RX(15), RX(11)  
RX(33) 2 Y + 2 AA ==> V



V  
YIELD 89%

RX(15) RCT Y 563-41-7

STAGE(1)

RGT AB 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON 1 hour, room temperature

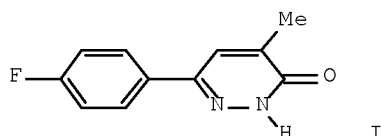
STAGE(2)

RCT AA 110-15-6  
SOL 123-91-1 Dioxane  
CON SUBSTAGE(1) 6 hours, reflux  
SUBSTAGE(2) overnight, room temperature

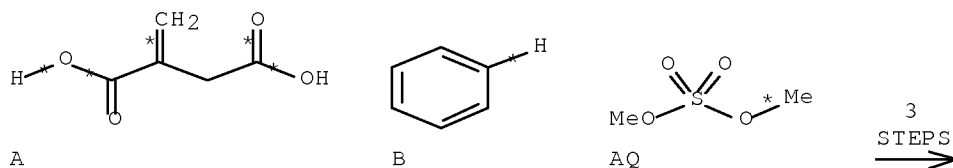
PRO I 851625-91-7

RX(11) RCT I 851625-91-7  
RGT S 7487-94-7 HgCl2  
PRO V 851625-88-2  
SOL 67-56-1 MeOH, 68-12-2 DMF  
CON 24 hours, room temperature

L91 ANSWER 7 OF 30 CASREACT COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 142:261502 CASREACT Full-text  
TITLE: Synthesis and hypotensive activity of some  
6-(substituted  
aryl)-4-methyl-2,3-dihydropyridazin-3-ones  
AUTHOR(S): Siddiqui, Anees A.; Wani, Sachin M.  
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Faculty of  
Pharmacy, Hamdard University, New Delhi, 110 062,  
India  
SOURCE: Indian Journal of Chemistry, Section B: Organic  
Chemistry Including Medicinal Chemistry (2004),  
43B(7), 1574-1579  
CODEN: IJSBDB; ISSN: 0376-4699  
PUBLISHER: National Institute of Science Communication  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

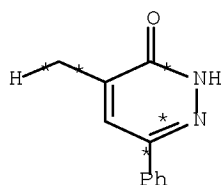


REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

$$\text{RX(101)} \quad \text{A} + \text{B} + \text{AO} \implies \text{BN}$$




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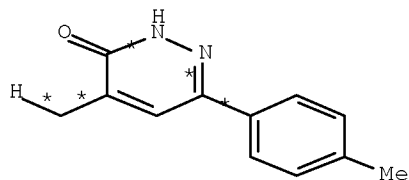
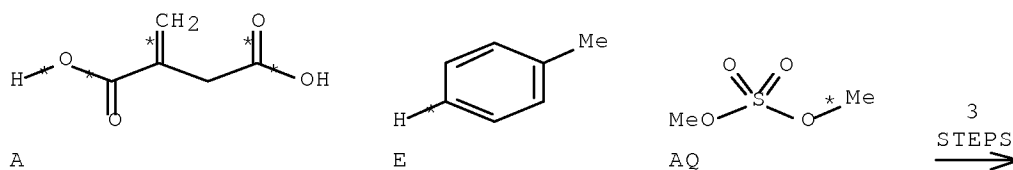
BN  
YIELD 65%

RX(1) RCT A 97-65-4, B 71-43-2  
RGT D 7446-70-0 AlCl3  
PRO C 15732-75-9  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) reflux  
SUBSTAGE(2) 4 hours, reflux

RX(21) RCT C 15732-75-9, AQ 77-78-1  
RGT AS 584-08-7 K2CO3  
PRO AR 148903-67-7  
SOL 75-05-8 MeCN  
CON 4 hours, reflux

RX(41) RCT AR 148903-67-7  
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4  
PRO BN 13300-09-9  
SOL 67-56-1 MeOH  
CON 8 hours, reflux

RX(102) OF 120 COMPOSED OF RX(2), RX(22), RX(42)  
RX(102) A + E + AQ ==> BR



BR  
YIELD 80%

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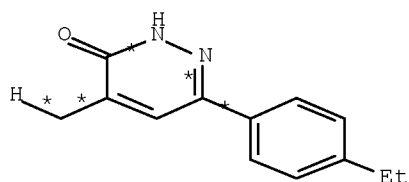
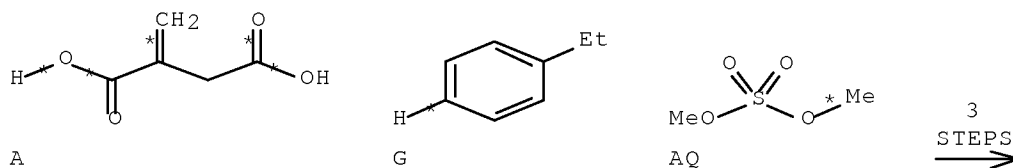
RX(2) RCT A 97-65-4, E 108-88-3  
 RGT D 7446-70-0 AlCl3  
 PRO F 19340-33-1  
 SOL 71-43-2 Benzene  
 CON SUBSTAGE(1) reflux  
 SUBSTAGE(2) 4 hours, reflux

RX(22) RCT F 19340-33-1, AQ 77-78-1  
 RGT AS 584-08-7 K2CO3  
 PRO AU 845961-24-2  
 SOL 75-05-8 MeCN  
 CON 4 hours, reflux

RX(42) RCT AU 845961-24-2  
 RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4  
 PRO BR 21004-61-5  
 SOL 67-56-1 MeOH  
 CON 8 hours, reflux

RX(103) OF 120 COMPOSED OF RX(3), RX(23), RX(43)

RX(103) A + G + AQ ==> BS



BS  
 YIELD 75%

RX(3) RCT A 97-65-4, G 100-41-4  
 RGT D 7446-70-0 AlCl3  
 PRO H 118540-59-3  
 SOL 71-43-2 Benzene  
 CON SUBSTAGE(1) reflux  
 SUBSTAGE(2) 4 hours, reflux

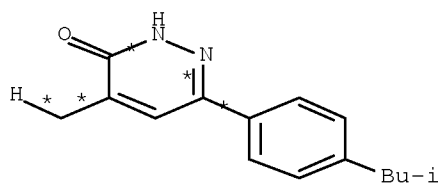
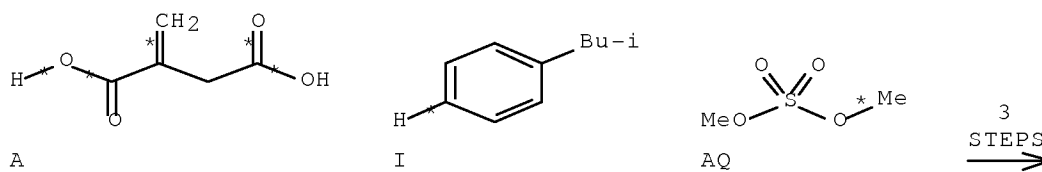
RX(23) RCT H 118540-59-3, AQ 77-78-1  
 RGT AS 584-08-7 K2CO3

10/595943

PRO AV 845961-25-3  
SOL 75-05-8 MeCN  
CON 4 hours, reflux

RX(43) RCT AV 845961-25-3  
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4  
PRO BS 845961-17-3  
SOL 67-56-1 MeOH  
CON 8 hours, reflux

RX(104) OF 120 COMPOSED OF RX(4), RX(24), RX(44)  
RX(104) A + I + AQ ==> BT



BT  
YIELD 72%

RX(4) RCT A 97-65-4, I 538-93-2  
RGT D 7446-70-0 AlCl3  
PRO J 845961-43-5  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) reflux  
SUBSTAGE(2) 4 hours, reflux

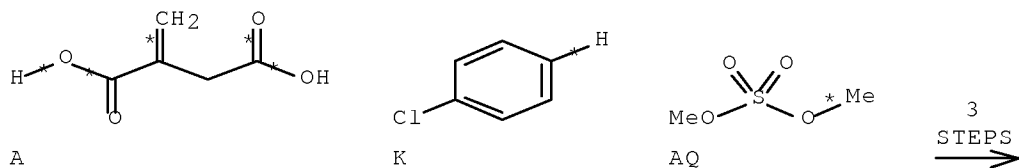
RX(24) RCT J 845961-43-5, AQ 77-78-1  
RGT AS 584-08-7 K2CO3  
PRO AW 845961-26-4  
SOL 75-05-8 MeCN  
CON 4 hours, reflux

RX(44) RCT AW 845961-26-4  
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4  
PRO BT 845961-18-4  
SOL 67-56-1 MeOH  
CON 8 hours, reflux

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RX(105) OF 120 COMPOSED OF RX(5), RX(25), RX(45)

RX(105) A + K + AQ ==> BU



BU  
YIELD 66%

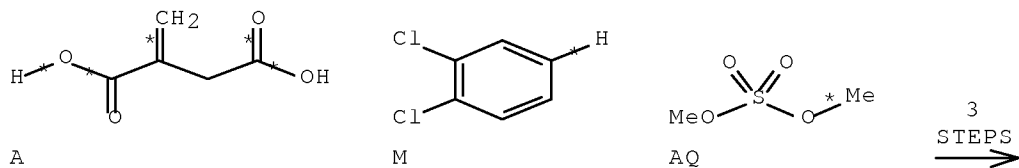
RX(5) RCT A 97-65-4, K 108-90-7  
RGT D 7446-70-0 AlCl3  
PRO L 58182-59-5  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) reflux  
SUBSTAGE(2) 4 hours, reflux

RX(25) RCT L 58182-59-5, AQ 77-78-1  
RGT AS 584-08-7 K2CO3  
PRO AX 845961-27-5  
SOL 75-05-8 MeCN  
CON 4 hours, reflux

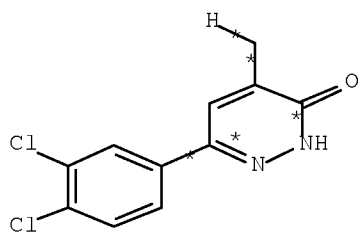
RX(45) RCT AX 845961-27-5  
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4  
PRO BU 32193-12-7  
SOL 67-56-1 MeOH  
CON 8 hours, reflux

RX(106) OF 120 COMPOSED OF RX(6), RX(26), RX(46)

RX(106) A + M + AQ ==> BV



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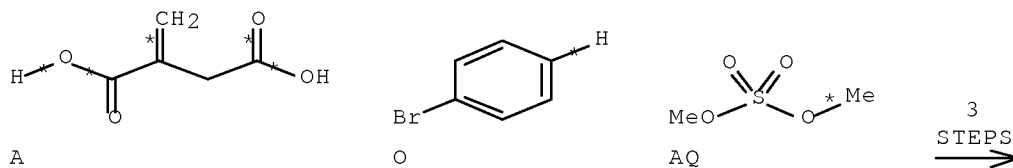
BV  
YIELD 65%

RX(6) RCT A 97-65-4, M 95-50-1  
RGT D 7446-70-0 AlCl3  
PRO N 191018-61-8  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) reflux  
SUBSTAGE(2) 4 hours, reflux

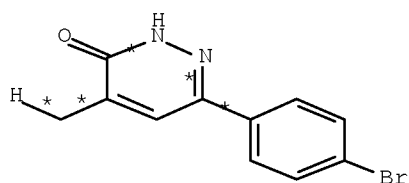
RX(26) RCT N 191018-61-8, AQ 77-78-1  
RGT AS 584-08-7 K2CO3  
PRO AY 845961-28-6  
SOL 75-05-8 MeCN  
CON 4 hours, reflux

RX(46) RCT AY 845961-28-6  
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4  
PRO BV 845961-19-5  
SOL 67-56-1 MeOH  
CON 8 hours, reflux

RX(107) OF 120 COMPOSED OF RX(7), RX(27), RX(47)  
RX(107) A + O + AQ ==> BW



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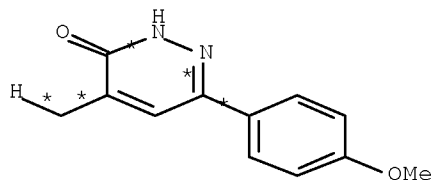
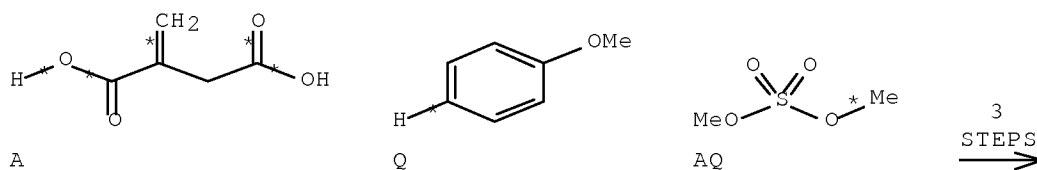
BW  
YIELD 68%

RX(7) RCT A 97-65-4, O 108-86-1  
RGT D 7446-70-0 AlCl3  
PRO P 101973-98-2  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) reflux  
SUBSTAGE(2) 4 hours, reflux

RX(27) RCT P 101973-98-2, AQ 77-78-1  
RGT AS 584-08-7 K2CO3  
PRO AZ 845961-29-7  
SOL 75-05-8 MeCN  
CON 4 hours, reflux

RX(47) RCT AZ 845961-29-7  
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4  
PRO BW 21004-64-8  
SOL 67-56-1 MeOH  
CON 8 hours, reflux

RX(108) OF 120 COMPOSED OF RX(8), RX(28), RX(48)  
RX(108) A + Q + AQ ==> BX



BX  
YIELD 75%

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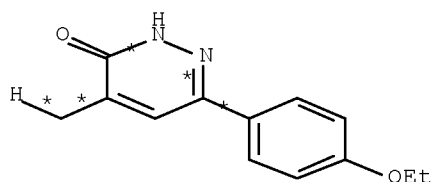
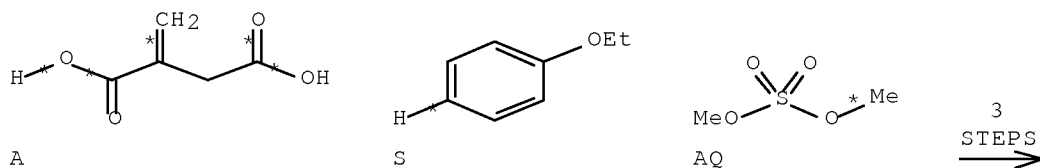
RX(8) RCT A 97-65-4, Q 100-66-3  
 RGT D 7446-70-0 AlCl3  
 PRO R 101973-94-8  
 SOL 71-43-2 Benzene  
 CON SUBSTAGE(1) reflux  
 SUBSTAGE(2) 4 hours, reflux

RX(28) RCT R 101973-94-8, AQ 77-78-1  
 RGT AS 584-08-7 K2CO3  
 PRO BA 845961-30-0  
 SOL 75-05-8 MeCN  
 CON 4 hours, reflux

RX(48) RCT BA 845961-30-0  
 RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4  
 PRO BX 28657-53-6  
 SOL 67-56-1 MeOH  
 CON 8 hours, reflux

RX(109) OF 120 COMPOSED OF RX(9), RX(29), RX(49)

RX(109) A + S + AQ ==> BY



BY  
 YIELD 72%

RX(9) RCT A 97-65-4, S 103-73-1  
 RGT D 7446-70-0 AlCl3  
 PRO T 845961-44-6  
 SOL 71-43-2 Benzene  
 CON SUBSTAGE(1) reflux  
 SUBSTAGE(2) 4 hours, reflux

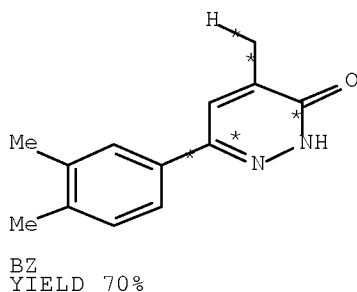
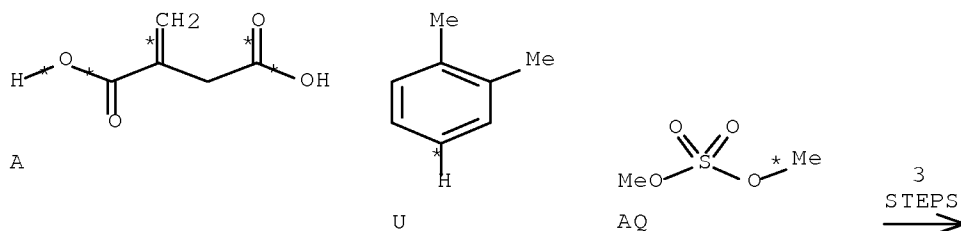
RX(29) RCT T 845961-44-6, AQ 77-78-1  
 RGT AS 584-08-7 K2CO3

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PRO BB 845961-31-1  
SOL 75-05-8 MeCN  
CON 4 hours, reflux

RX(49) RCT BB 845961-31-1  
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4  
PRO BY 845961-20-8  
SOL 67-56-1 MeOH  
CON 8 hours, reflux

RX(110) OF 120 COMPOSED OF RX(10), RX(30), RX(50)  
RX(110) A + U + AQ ==> BZ



RX(10) RCT A 97-65-4, U 95-47-6  
RGT D 7446-70-0 AlCl3  
PRO V 101973-97-1  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) reflux  
SUBSTAGE(2) 4 hours, reflux

RX(30) RCT V 101973-97-1, AQ 77-78-1  
RGT AS 584-08-7 K2CO3  
PRO BC 845961-32-2  
SOL 75-05-8 MeCN  
CON 4 hours, reflux

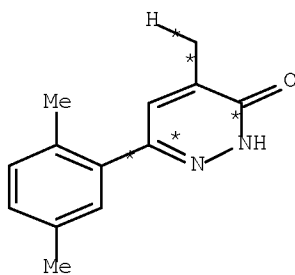
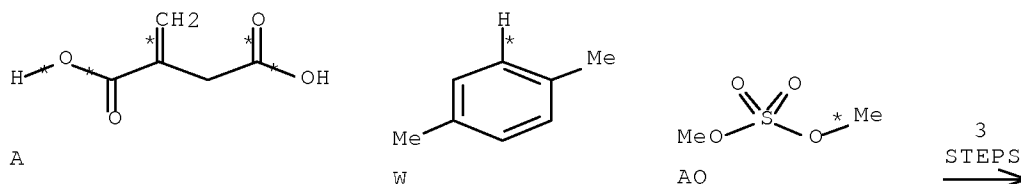
RX(50) RCT BC 845961-32-2  
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4



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PRO BZ 64262-76-6  
SOL 67-56-1 MeOH  
CON 8 hours, reflux

RX(111) OF 120 COMPOSED OF RX(11), RX(31), RX(51)  
RX(111) A + W + AQ ==> CA



CA  
YIELD 66%

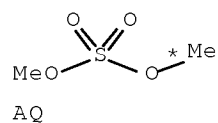
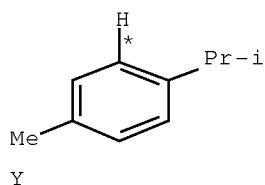
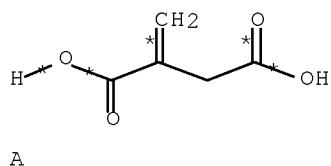
RX(11) RCT A 97-65-4, W 106-42-3  
RGT D 7446-70-0 AlCl3  
PRO X 118540-58-2  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) reflux  
SUBSTAGE(2) 4 hours, reflux

RX(31) RCT X 118540-58-2, AQ 77-78-1  
RGT AS 584-08-7 K2CO3  
PRO BD 845961-33-3  
SOL 75-05-8 MeCN  
CON 4 hours, reflux

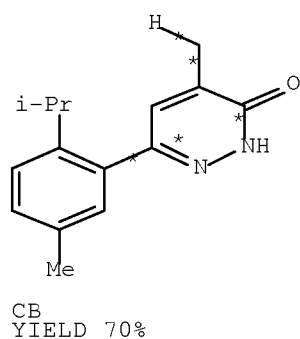
RX(51) RCT BD 845961-33-3  
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4  
PRO CA 64262-78-8  
SOL 67-56-1 MeOH  
CON 8 hours, reflux

RX(112) OF 120 COMPOSED OF RX(12), RX(32), RX(52)  
RX(112) A + Y + AQ ==> CB

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3  
STEPS  
→



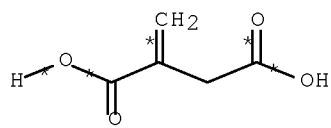
RX(12) RCT A 97-65-4, Y 99-87-6  
RGT D 7446-70-0 AlCl3  
PRO Z 845961-45-7  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) reflux  
SUBSTAGE(2) 4 hours, reflux

RX(32) RCT Z 845961-45-7, AQ 77-78-1  
RGT AS 584-08-7 K2CO3  
PRO BE 845961-34-4  
SOL 75-05-8 MeCN  
CON 4 hours, reflux

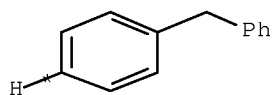
RX(52) RCT BE 845961-34-4  
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4  
PRO CB 845961-21-9  
SOL 67-56-1 MeOH  
CON 8 hours, reflux

RX(113) OF 120 COMPOSED OF RX(13), RX(33), RX(53)  
RX(113) A + AA + AQ ==> CC

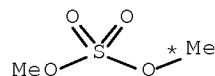
10/595943



A

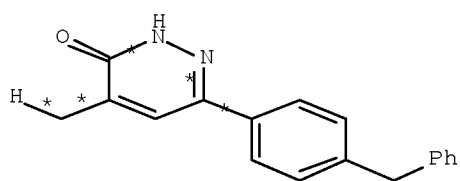


AA



AQ

3  
STEPS  
→



CC  
YIELD 66%

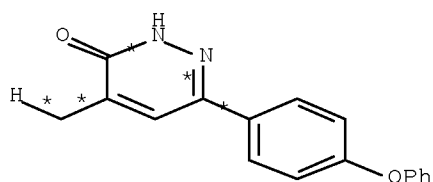
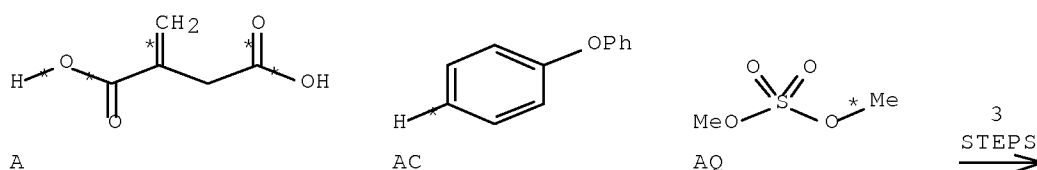
RX(13)     RCT    A 97-65-4, AA 101-81-5  
             RGT    D 7446-70-0 AlCl3  
             PRO    AB 845961-46-8  
             SOL    71-43-2 Benzene  
             CON    SUBSTAGE(1) reflux  
                     SUBSTAGE(2) 4 hours, reflux

RX(33)     RCT    AB 845961-46-8, AQ 77-78-1  
             RGT    AS 584-08-7 K2CO3  
             PRO    BF 845961-35-5  
             SOL    75-05-8 MeCN  
             CON    4 hours, reflux

RX(53)     RCT    BF 845961-35-5  
             RGT    BO 127-09-3 AcONa, BP 302-01-2 N2H4  
             PRO    CC 845961-22-0  
             SOL    67-56-1 MeOH  
             CON    8 hours, reflux

RX(114) OF 120 COMPOSED OF RX(14), RX(34), RX(54)  
RX(114)    A   +   AC   +   AQ   ==>   CD

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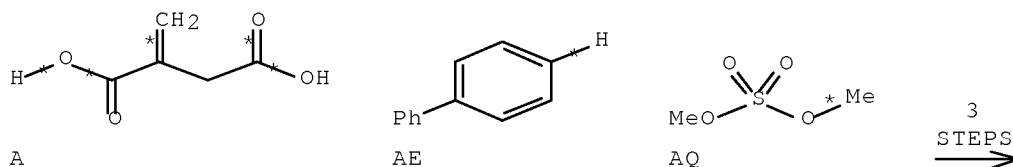
CD  
YIELD 71%

RX(14) RCT A 97-65-4, AC 101-84-8  
RGT D 7446-70-0 AlCl3  
PRO AD 58182-60-8  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) reflux  
SUBSTAGE(2) 4 hours, reflux

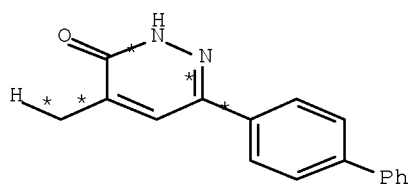
RX(34) RCT AD 58182-60-8, AQ 77-78-1  
RGT AS 584-08-7 K2CO3  
PRO BG 845961-36-6  
SOL 75-05-8 MeCN  
CON 4 hours, reflux

RX(54) RCT BG 845961-36-6  
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4  
PRO CD 68195-42-6  
SOL 67-56-1 MeOH  
CON 8 hours, reflux

RX(115) OF 120 COMPOSED OF RX(15), RX(35), RX(55)  
RX(115) A + AE + AQ ==> CE



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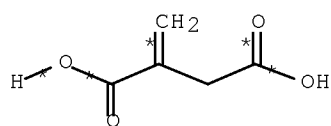
CE  
YIELD 76%

RX(15) RCT A 97-65-4, AE 92-52-4  
RGT D 7446-70-0 AlCl3  
PRO AF 19340-35-3  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) reflux  
SUBSTAGE(2) 4 hours, reflux

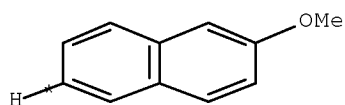
RX(35) RCT AF 19340-35-3, AQ 77-78-1  
RGT AS 584-08-7 K2CO3  
PRO BH 845961-37-7  
SOL 75-05-8 MeCN  
CON 4 hours, reflux

RX(55) RCT BH 845961-37-7  
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4  
PRO CE 21004-63-7  
SOL 67-56-1 MeOH  
CON 8 hours, reflux

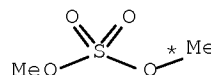
RX(116) OF 120 COMPOSED OF RX(16), RX(36), RX(56)  
RX(116) A + AG + AQ ==> CF



A



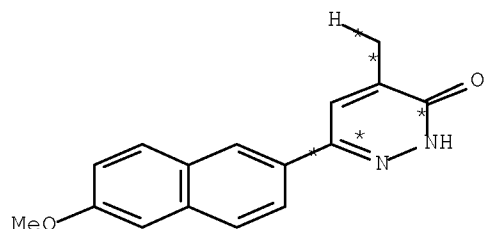
AG



AQ

3  
STEPS  
→

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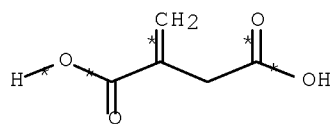
CF  
YIELD 57%

RX(16)      RCT    A 97-65-4, AG 93-04-9  
              RGT    D 7446-70-0 AlCl3  
              PRO    AH 845961-47-9  
              SOL    71-43-2 Benzene  
              CON    SUBSTAGE(1) reflux  
                      SUBSTAGE(2) 4 hours, reflux

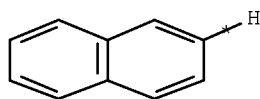
RX(36)      RCT    AH 845961-47-9, AQ 77-78-1  
              RGT    AS 584-08-7 K2CO3  
              PRO    BI 845961-38-8  
              SOL    75-05-8 MeCN  
              CON    4 hours, reflux

RX(56)      RCT    BI 845961-38-8  
              RGT    BO 127-09-3 AcONa, BP 302-01-2 N2H4  
              PRO    CF 845961-23-1  
              SOL    67-56-1 MeOH  
              CON    8 hours, reflux

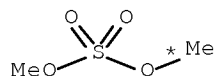
RX(117) OF 120 COMPOSED OF RX(17), RX(37), RX(57)  
RX(117)    A + AI + AQ ==> CG



A



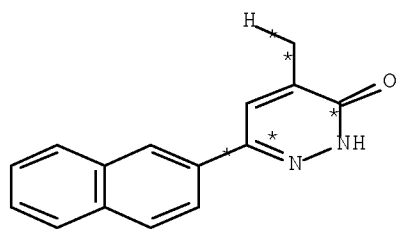
AI



AQ

3  
STEPS  
→

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CG  
YIELD 54%

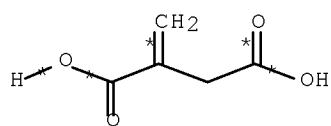
RX(17) RCT A 97-65-4, AI 91-20-3  
RGT D 7446-70-0 AlCl3  
PRO AJ 60186-01-8  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) reflux  
SUBSTAGE(2) 4 hours, reflux

RX(37) RCT AJ 60186-01-8, AQ 77-78-1  
RGT AS 584-08-7 K2CO3  
PRO BJ 845961-39-9  
SOL 75-05-8 MeCN  
CON 4 hours, reflux

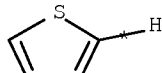
RX(57) RCT BJ 845961-39-9  
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4  
PRO CG 28734-27-2  
SOL 67-56-1 MeOH  
CON 8 hours, reflux

RX(118) OF 120 COMPOSED OF RX(18), RX(38), RX(58)

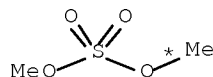
RX(118) A + AK + AQ ==> CH



A

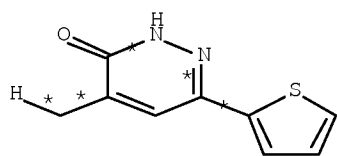


AK



AQ

3  
STEPS  
→



CH  
YIELD 56%

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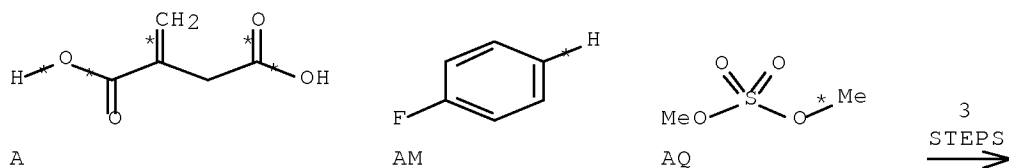
RX(18) RCT A 97-65-4, AK 110-02-1  
 RGT D 7446-70-0 AlCl3  
 PRO AL 845961-48-0  
 SOL 71-43-2 Benzene  
 CON SUBSTAGE(1) reflux  
 SUBSTAGE(2) 4 hours, reflux

RX(38) RCT AL 845961-48-0, AQ 77-78-1  
 RGT AS 584-08-7 K2CO3  
 PRO BK 845961-40-2  
 SOL 75-05-8 MeCN  
 CON 4 hours, reflux

RX(58) RCT BK 845961-40-2  
 RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4  
 PRO CH 28657-57-0  
 SOL 67-56-1 MeOH  
 CON 8 hours, reflux

RX(119) OF 120 COMPOSED OF RX(19), RX(39), RX(59)

RX(119) A + AM + AQ ==> CI



RX(19) RCT A 97-65-4, AM 462-06-6  
 RGT D 7446-70-0 AlCl3  
 PRO AN 58182-61-9  
 SOL 71-43-2 Benzene  
 CON SUBSTAGE(1) reflux  
 SUBSTAGE(2) 4 hours, reflux

RX(39) RCT AN 58182-61-9, AQ 77-78-1  
 RGT AS 584-08-7 K2CO3

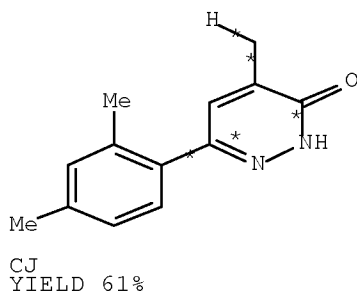
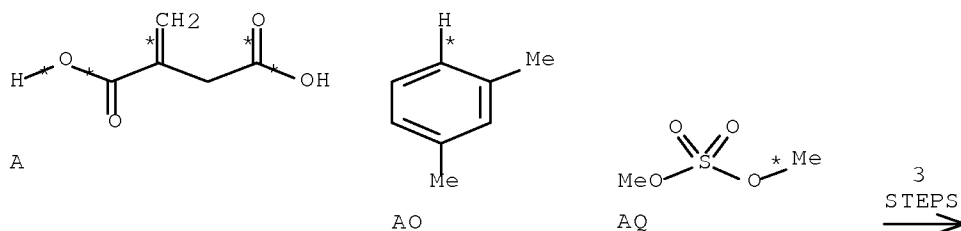


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PRO BL 845961-41-3  
SOL 75-05-8 MeCN  
CON 4 hours, reflux

RX(59) RCT BL 845961-41-3  
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4  
PRO CI 68612-32-8  
SOL 67-56-1 MeOH  
CON 8 hours, reflux

RX(120) OF 120 COMPOSED OF RX(20), RX(40), RX(60)  
RX(120) A + AO + AQ ==> CJ



RX(20) RCT A 97-65-4, AO 108-38-3  
RGT D 7446-70-0 AlCl3  
PRO AP 101973-96-0  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) reflux  
SUBSTAGE(2) 4 hours, reflux

RX(40) RCT AP 101973-96-0, AQ 77-78-1  
RGT AS 584-08-7 K2CO3  
PRO BM 845961-42-4  
SOL 75-05-8 MeCN  
CON 4 hours, reflux

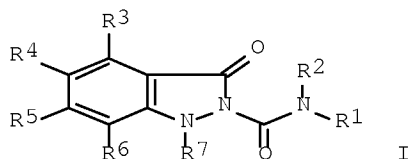
RX(60) RCT BM 845961-42-4  
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4

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PRO CJ 64262-77-7  
SOL 67-56-1 MeOH  
CON 8 hours, reflux

L91 ANSWER 8 OF 30 CASREACT COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 141:395549 CASREACT Full-text  
TITLE: Preparation of 3-oxo-1,3-dihydro-indazole-2-carboxylic  
acid amide derivatives as phospholipase inhibitors  
INVENTOR(S): Eacho, Patrick Irving; Foxworthy-Mason, Patricia Sue;  
Lin, Ho-Shen; Lopez, Jose Eduardo; Mosior, Marian  
Kazimierz; Richett, Michael Enrico  
PATENT ASSIGNEE(S): Eli Lilly and Company, USA  
SOURCE: PCT Int. Appl., 131 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2004093872	A1	20041104	WO 2004-US6092	20040325
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1610779	A1	20060104	EP 2004-723448	20040325
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
US 20060211755	A1	20060921	US 2005-544910	20050810
PRIORITY APPLN. INFO.:			US 2003-459362P	20030331
			WO 2004-US6092	20040325
OTHER SOURCE(S):			MARPAT 141:395549	
GI				



AB Title compds. I [R1 = alkyl, haloalkyl, alkenyl, alkynyl, etc.; R2 = H; R3-6 = H, alk(en/yn)yl, haloalkyl, etc.; R7 = H, alk(en/yn)yl, haloalkyl, etc.] are prepared For instance, 3-oxo-1,3-dihydroindazole-2-carboxylic acid N-propylamide is prepared from Pr isocyanate and 1,2-dihydroindazol-3-one.

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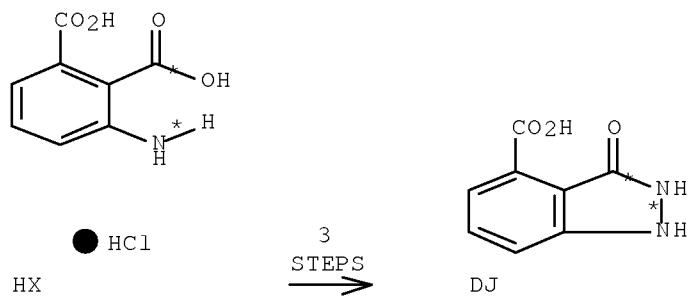
Selected compds. exhibited inhibitory activity toward endothelial lipase; IC50 11.39 - 45.14 nM. I are useful for the treatment of hepatic lipase and/or endothelial lipase-mediated diseases.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

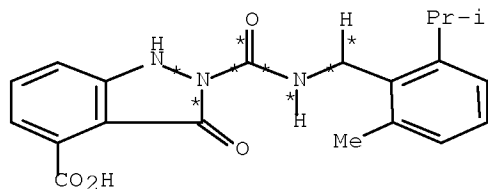
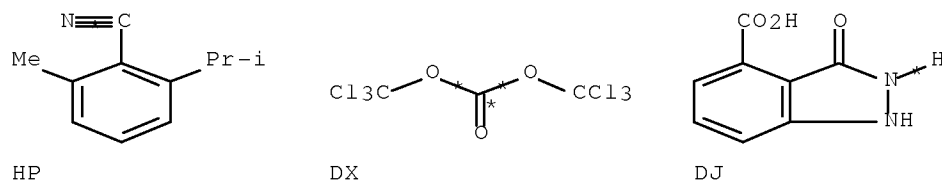
RX(365) OF 500 COMPOSED OF REACTION SEQUENCE RX(115), RX(65)  
AND REACTION SEQUENCE RX(107), RX(121), RX(65)

... HX ==> DJ...

...HP + DX + DJ ==> EP



START NEXT REACTION SEQUENCE



YIELD 69%

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RX(115) RCT HX 6946--22-1

STAGE(1)

RGT DP 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON 10 minutes, -10 deg C

STAGE(2)

RGT DQ 7632-00-0 NaNO2  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) -10 deg C  
SUBSTAGE(2) 1 hour, -10 deg C

STAGE(3)

RGT DP 7647-01-0 HCl, DR 7772-99-8 SnCl2  
SOL 7732-18-5 Water, 7647-01-0 HCl  
CON SUBSTAGE(1) 15 minutes, -10 deg C  
SUBSTAGE(2) 30 minutes, -10 deg C  
SUBSTAGE(3) -10 deg C -> room temperature  
SUBSTAGE(4) 16 hours, room temperature

PRO DJ 7384-17-0

NTE incremental addition of the diazotized solution in third stage

RX(107) RCT HP 786677-15-4

STAGE(1)

RGT BS 16940-66-2 NaBH4  
SOL 60-29-7 Et2O  
CON SUBSTAGE(1) 16 hours, room temperature  
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RGT BV 67-56-1 MeOH  
CON 0 deg C

PRO BX 786677-17-6

RX(121) RCT BX 786677-17-6, DX 32315-10-9

RGT EA 20734-58-1 Proton sponge  
PRO EO 787580-99-8  
SOL 75-09-2 CH2Cl2  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 15 minutes, room temperature

RX(65) RCT DJ 7384-17-0, EO 787580-99-8

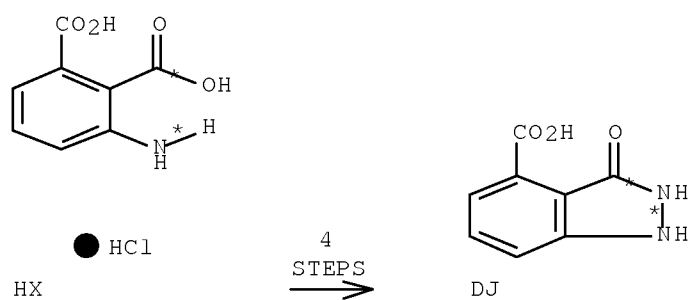
PRO EP 787580-05-6  
SOL 109-99-9 THF  
CON 16 hours, room temperature  
NTE chemoselective

RX(419) OF 500 COMPOSED OF REACTION SEQUENCE RX(115), RX(65)  
AND REACTION SEQUENCE RX(106), RX(107), RX(121), RX(65)

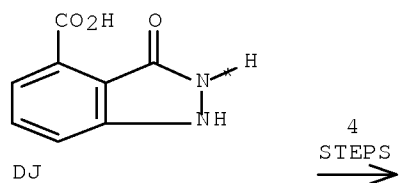
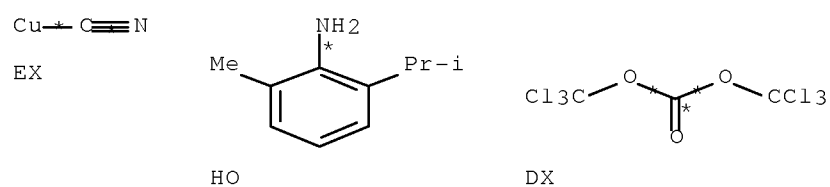
... HX ==> DJ...

...EX + HO + DX + DJ ==> EP

10/595943



START NEXT REACTION SEQUENCE



EP  
YIELD 69%

RX(115) RCT HX 6946-22-1

STAGE(1)

RGT DP 7647-01-0 HCl

SOL 7732-18-5 Water

CON 10 minutes, -10 deg C

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STAGE(2)

RGT DQ 7632-00-0 NaNO2  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) -10 deg C  
SUBSTAGE(2) 1 hour, -10 deg C

STAGE(3)

RGT DP 7647-01-0 HCl, DR 7772-99-8 SnCl2  
SOL 7732-18-5 Water, 7647-01-0 HCl  
CON SUBSTAGE(1) 15 minutes, -10 deg C  
SUBSTAGE(2) 30 minutes, -10 deg C  
SUBSTAGE(3) -10 deg C -> room temperature  
SUBSTAGE(4) 16 hours, room temperature

PRO DJ 7384-17-0

NTE incremental addition of the diazotized solution in third stage

RX(106) RCT EX 544-92-3

STAGE(1)

RGT FA 594-70-7 Propane, 2-methyl-2-nitro-  
SOL 67-68-5 DMSO  
CON 60 deg C

STAGE(2)

RCT HO 5266-85-3  
SOL 67-68-5 DMSO  
CON SUBSTAGE(1) 60 deg C  
SUBSTAGE(2) 1 hour, 60 deg C  
SUBSTAGE(3) 60 deg C -> 45 deg C

STAGE(3)

RGT DP 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 5 minutes, 45 deg C  
SUBSTAGE(2) 45 deg C -> room temperature

PRO HP 786677-15-4

RX(107) RCT HP 786677-15-4

STAGE(1)

RGT BS 16940-66-2 NaBH4  
SOL 60-29-7 Et2O  
CON SUBSTAGE(1) 16 hours, room temperature  
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RGT BV 67-56-1 MeOH  
CON 0 deg C

PRO BX 786677-17-6

RX(121) RCT BX 786677-17-6, DX 32315-10-9

RGT EA 20734-58-1 Proton sponge  
PRO EO 787580-99-8  
SOL 75-09-2 CH2Cl2  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 15 minutes, room temperature

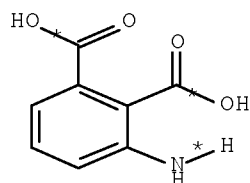
10/595943

RX(65) RCT DJ 7384-17-0, EO 787580-99-8  
 PRO EP 787580-05-6  
 SOL 109-99-9 THF  
 CON 16 hours, room temperature  
 NTE chemoselective

RX(436) OF 500 COMPOSED OF REACTION SEQUENCE RX(115), RX(142), RX(101)  
 AND REACTION SEQUENCE RX(107), RX(121), RX(101)

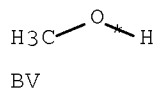
... HX + BV ==> HE...

...HP + DX + HE ==> HK



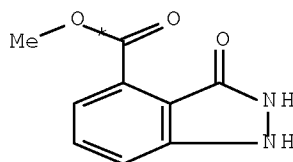
HX

● HCl



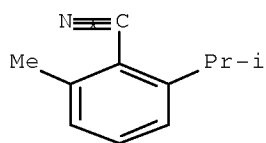
BV

3  
STEPS  
→

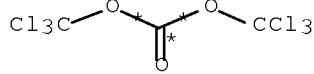


HE

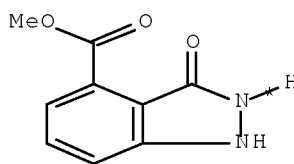
START NEXT REACTION SEQUENCE



HP

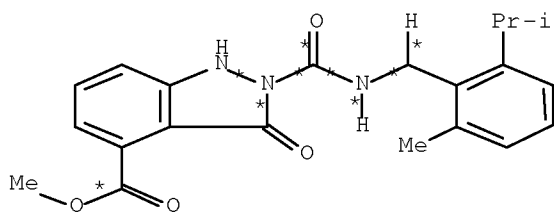


DX



HE

3  
STEPS  
→



HK  
YIELD 85%

RX(115) RCT HX 6946-22-1

STAGE(1)  
 RGT DP 7647-01-0 HCl  
 SOL 7732-18-5 Water  
 CON 10 minutes, -10 deg C

STAGE(2)  
 RGT DQ 7632-00-0 NaNO2  
 SOL 7732-18-5 Water  
 CON SUBSTAGE(1) -10 deg C  
 SUBSTAGE(2) 1 hour, -10 deg C

STAGE(3)  
 RGT DP 7647-01-0 HCl, DR 7772-99-8 SnCl2  
 SOL 7732-18-5 Water, 7647-01-0 HCl  
 CON SUBSTAGE(1) 15 minutes, -10 deg C  
 SUBSTAGE(2) 30 minutes, -10 deg C  
 SUBSTAGE(3) -10 deg C -> room temperature  
 SUBSTAGE(4) 16 hours, room temperature

PRO DJ 7384-17-0  
 NTE incremental addition of the diazotized solution in third stage

RX(142) RCT DJ 7384-17-0, BV 67-56-1  
 RGT DP 7647-01-0 HCl  
 PRO HE 787581-35-5  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON 4 hours, room temperature -> reflux

RX(107) RCT HP 786677-15-4

STAGE(1)  
 RGT BS 16940-66-2 NaBH4  
 SOL 60-29-7 Et2O  
 CON SUBSTAGE(1) 16 hours, room temperature  
 SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)  
 RGT BV 67-56-1 MeOH  
 CON 0 deg C

PRO BX 786677-17-6

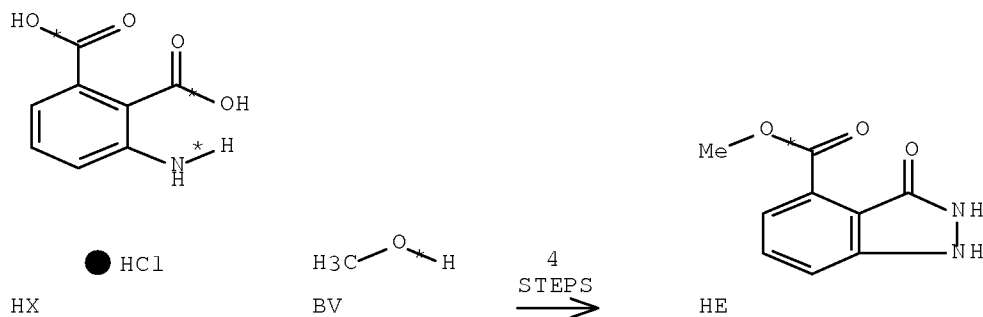
RX(121) RCT BX 786677-17-6, DX 32315-10-9  
 RGT EA 20734-58-1 Proton sponge  
 PRO EO 787580-99-8  
 SOL 75-09-2 CH2Cl2  
 CON SUBSTAGE(1) 0 deg C  
 SUBSTAGE(2) 15 minutes, room temperature

RX(101) RCT EO 787580-99-8, HE 787581-35-5  
 PRO HK 787580-78-3  
 SOL 68-12-2 DMF  
 CON 3 hours, room temperature

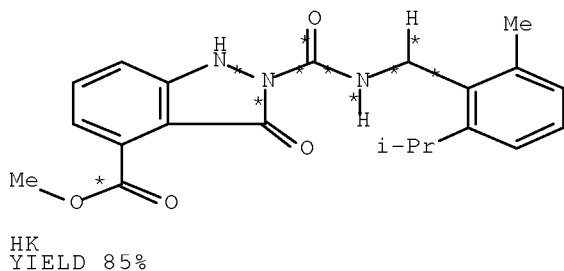
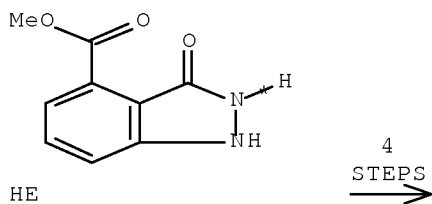
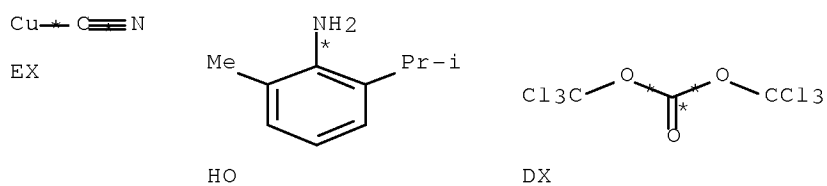


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RX(451) OF 500 COMPOSED OF REACTION SEQUENCE RX(115), RX(142), RX(101)  
 AND REACTION SEQUENCE RX(106), RX(107), RX(121), RX(101)  
 ... RX + BV ==> HE...  
 ...EX + HO + DX + HE ==> HK



START NEXT REACTION SEQUENCE



RX(115) RCT HX 6946-22-1

## STAGE(1)

RGT DP 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON 10 minutes, -10 deg C

## STAGE(2)

RGT DQ 7632-00-0 NaNO2  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) -10 deg C  
SUBSTAGE(2) 1 hour, -10 deg C

## STAGE(3)

RGT DP 7647-01-0 HCl, DR 7772-99-8 SnCl2  
SOL 7732-18-5 Water, 7647-01-0 HCl  
CON SUBSTAGE(1) 15 minutes, -10 deg C  
SUBSTAGE(2) 30 minutes, -10 deg C  
SUBSTAGE(3) -10 deg C -> room temperature  
SUBSTAGE(4) 16 hours, room temperature

PRO DJ 7384-17-0

NTE incremental addition of the diazotized solution in third stage

RX(142) RCT DJ 7384-17-0, BV 67-56-1

RGT DP 7647-01-0 HCl  
PRO HE 787581-35-5  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON 4 hours, room temperature -> reflux

RX(106) RCT EX 544-92-3

## STAGE(1)

RGT FA 594-70-7 Propane, 2-methyl-2-nitro-  
SOL 67-68-5 DMSO  
CON 60 deg C

## STAGE(2)

RCT HO 5266-85-3  
SOL 67-68-5 DMSO  
CON SUBSTAGE(1) 60 deg C  
SUBSTAGE(2) 1 hour, 60 deg C  
SUBSTAGE(3) 60 deg C -> 45 deg C

## STAGE(3)

RGT DP 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 5 minutes, 45 deg C  
SUBSTAGE(2) 45 deg C -> room temperature

PRO HP 786677-15-4

RX(107) RCT HP 786677-15-4

## STAGE(1)

RGT BS 16940-66-2 NaBH4

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SOL 60-29-7 Et2O  
CON SUBSTAGE(1) 16 hours, room temperature  
SUBSTAGE(2) room temperature -> 0 deg C

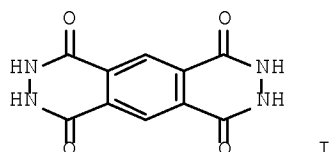
STAGE(2)  
RGT BV 67-56-1 MeOH  
CON 0 deg C

PRO BX 786677-17-6

RX(121) RCT BX 786677-17-6, DX 32315-10-9  
RGT EA 20734-58-1 Proton sponge  
PRO EO 787580-99-8  
SOL 75-09-2 CH2Cl2  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 15 minutes, room temperature

RX(101) RCT EO 787580-99-8, HE 787581-35-5  
PRO HK 787580-78-3  
SOL 68-12-2 DMF  
CON 3 hours, room temperature

L91 ANSWER 9 OF 30 CASREACT COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 141:306350 CASREACT Full-text  
TITLE: One- and three-dimensional coordination polymers  
containing organic ligands produced through in situ  
hydrothermal reactions  
AUTHOR(S): Hu, Xi-Xue; Pan, Cheng-Ling; Xu, Ji-Qing; Cui,  
Xiao-Bing; Yang, Guang-Di; Wang, Tie-Gang  
CORPORATE SOURCE: College of Chemistry and State Key Laboratory of  
Inorganic Synthesis and Preparative Chemistry, Jilin  
University, Changchun, 130023, Peop. Rep. China  
SOURCE: European Journal of Inorganic Chemistry (2004), (7),  
1566-1569  
CODEN: EJICFO; ISSN: 1434-1948  
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



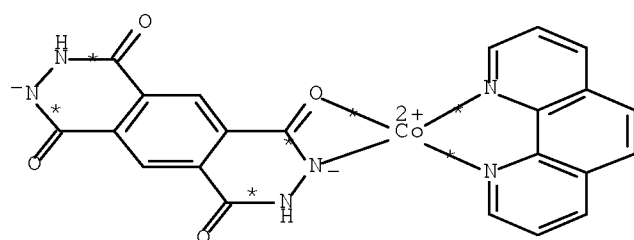
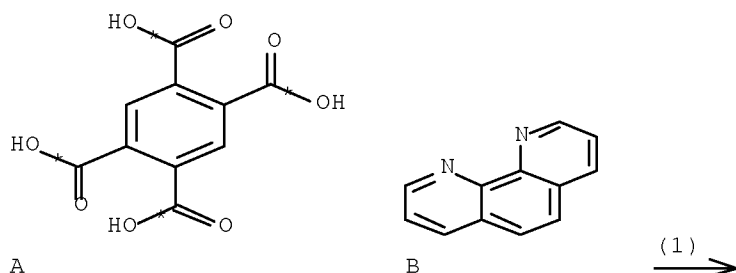
AB Two novel coordination polymers of cobalt(II), [Co( $\mu$ 3-H2bbh)(phen)]<sub>n</sub> (1) and [Co( $\mu$ 4-H2bbh)(H2O)]<sub>2n</sub> (2, phen = 1,10-phenanthroline; H4bbh = benzene-1,2,4,5-tetracarbo-1,2:4,5-dihydrazide, I), in which H2bbh ligands are in situ generated by an acylation reaction of H4bta (H4bta = benzene-1,2,4,5-tetracarboxylic acid) with hydrazine hydrate under hydrothermal conditions, were synthesized and structurally characterized. 1 Has a one-dimensional

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double-chain structure, while 2 has a three-dimensional network structure.  
Preliminary magnetic studies of 1 and 2 are reported.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 2 A + B ==> C

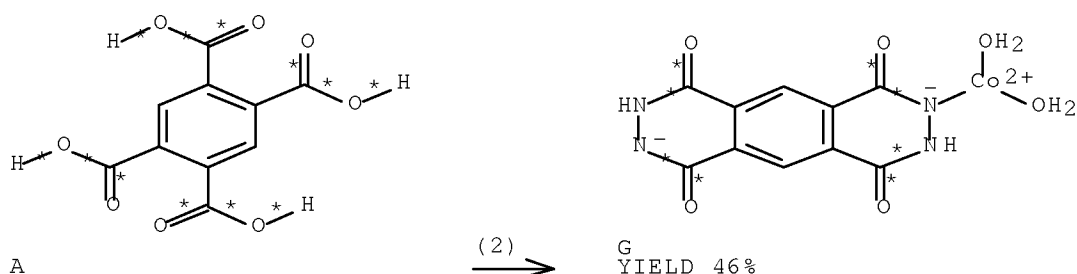


C  
YIELD 41%

RX(1) RCT A 89-05-4, B 66-71-7  
RGT D 302-01-2 N2H4, E 7646-79-9 CoCl2  
PRO C 681439-74-7  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 4 days, 170 deg C  
SUBSTAGE(2) 170 deg C -> room temperature  
NTE thermal, hydrothermal, Teflon-lined stainless steel autoclave  
used

RX(2) OF 2 A ==> G

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RX(2) RCT A 89-05-4  
 RGT D 302-01-2 N2H4, E 7646-79-9 CoCl2  
 PRO G 765313-22-2  
 SOL 7732-18-5 Water  
 CON SUBSTAGE(1) 4 days, 170 deg C  
 SUBSTAGE(2) 170 deg C -> room temperature  
 NTE thermal, hydrothermal, Teflon-lined stainless steel autoclave used

L91 ANSWER 10 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 141:225427 CASREACT [Full-text](#)

TITLE: Novel and efficient solid-phase synthesis of 4,6-disubstituted 4,5-dihydro-3(2H)-pyridazinone

AUTHOR(S): Tang, Jing; Huang, Xian

CORPORATE SOURCE: Dep. Chem., Zhejiang Univ., Hangzhou, 310 028, Peop. Rep. China

SOURCE: Journal of Chemical Research, Synopses (2003), (9), 599-600

CODEN: JRPSDC; ISSN: 0308-2342

PUBLISHER: Science Reviews

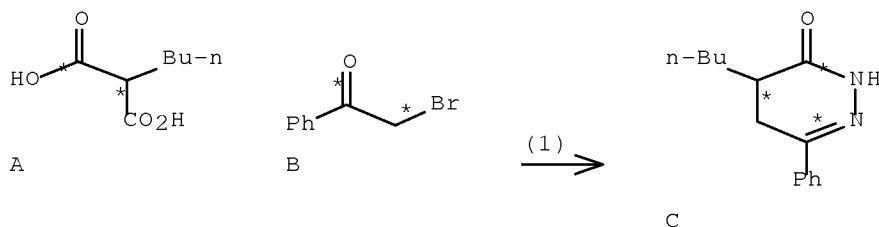
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The resin-bound 5-monosubstituted cyclic malonic ester was generated and reacted with an  $\alpha$ -bromoketone to give the corresponding 5,5-disubstituted cyclic malonic ester resin. Subsequent reaction with hydrazine resulted in cyclization with concomitant cleavage from the polymeric support to release the final products, 4,6-disubstituted 4,5-dihydro-3(2H)-pyridazinones, in good yield and high purity.

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 9 A + B ==> C



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RX(1)

STAGE(1)

RGT D 100-44-7D PhCH<sub>2</sub>Cl, E 19232-39-4 Butanoic acid, 3-oxo-, ethyl ester, ion(1-), sodium (1:1)

SOL 68-12-2 DMF

CON 16 hours, 80 deg C

STAGE(2)

RGT F 7647-14-5 NaCl

SOL 67-68-5 DMSO

CON 48 hours, 140 deg C

STAGE(3)

RCT A 534-59-8

RGT G 108-24-7 Ac<sub>2</sub>O, H 7664-93-9 H<sub>2</sub>SO<sub>4</sub>

SOL 7732-18-5 Water

STAGE(4)

RCT B 70-11-1

RGT I 127-09-3 AcONa, J 64-19-7 AcOH

SOL 68-12-2 DMF

CON SUBSTAGE(1) 1 hour, room temperature

SUBSTAGE(2) 24 hours, room temperature

STAGE(5)

RGT K 302-01-2 N<sub>2</sub>H<sub>4</sub>

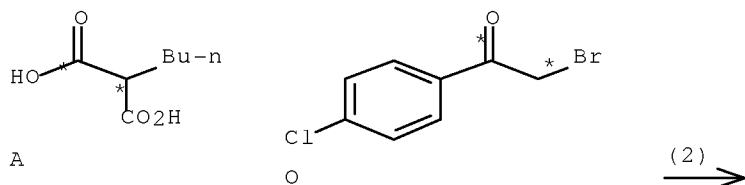
SOL 7732-18-5 Water, 68-12-2 DMF

CON 17 hours, room temperature

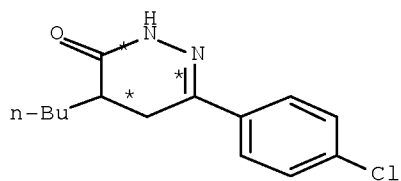
PRO C 746662-97-5

NTE solid-supported reagent, Merrifield resin used

RX(2) OF 9 A + O ==> P



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P

RX(2)

STAGE(1)

RGT D 100-44-7D PhCH<sub>2</sub>Cl, E 19232-39-4 Butanoic acid, 3-oxo-, ethyl ester, ion(1-), sodium (1:1)  
SOL 68-12-2 DMF  
CON 16 hours, 80 deg C

STAGE(2)

RGT F 7647-14-5 NaCl  
SOL 67-68-5 DMSO  
CON 48 hours, 140 deg C

STAGE(3)

RCT A 534-59-8  
RGT G 108-24-7 Ac<sub>2</sub>O, H 7664-93-9 H<sub>2</sub>SO<sub>4</sub>  
SOL 7732-18-5 Water

STAGE(4)

RCT O 536-38-9  
RGT I 127-09-3 AcONa, J 64-19-7 AcOH  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 1 hour, room temperature  
SUBSTAGE(2) 24 hours, room temperature

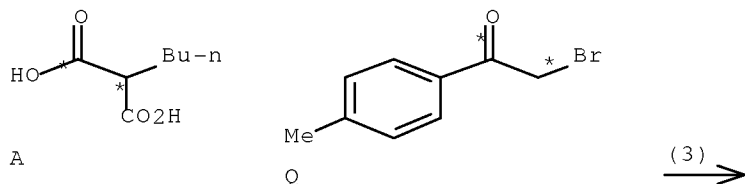
STAGE(5)

RGT K 302-01-2 N<sub>2</sub>H<sub>4</sub>  
SOL 7732-18-5 Water, 68-12-2 DMF  
CON 17 hours, room temperature

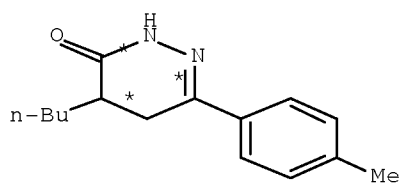
PRO P 746662-98-6

NTE solid-supported reagent, Merrifield resin used

RX(3) OF 9 A + Q ==> R



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R

RX(3)

STAGE(1)

RGT D 100-44-7D PhCH<sub>2</sub>Cl, E 19232-39-4 Butanoic acid, 3-oxo-, ethyl ester, ion(1-), sodium (1:1)  
SOL 68-12-2 DMF  
CON 16 hours, 80 deg C

STAGE(2)

RGT F 7647-14-5 NaCl  
SOL 67-68-5 DMSO  
CON 48 hours, 140 deg C

STAGE(3)

RCT A 534-59-8  
RGT G 108-24-7 Ac<sub>2</sub>O, H 7664-93-9 H<sub>2</sub>SO<sub>4</sub>  
SOL 7732-18-5 Water

STAGE(4)

RCT Q 619-41-0  
RGT I 127-09-3 AcONa, J 64-19-7 AcOH  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 1 hour, room temperature  
SUBSTAGE(2) 24 hours, room temperature

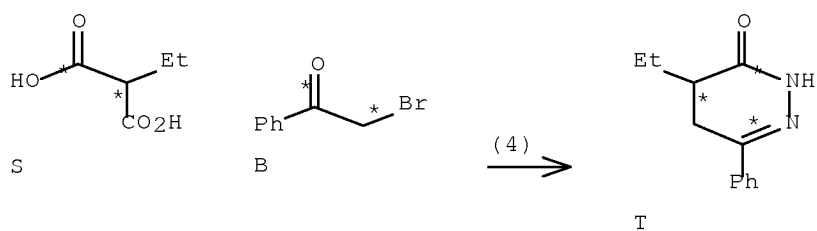
STAGE(5)

RGT K 302-01-2 N<sub>2</sub>H<sub>4</sub>  
SOL 7732-18-5 Water, 68-12-2 DMF  
CON 17 hours, room temperature

PRO R 746662-99-7

NTE solid-supported reagent, Merrifield resin used

RX(4) OF 9 S + B ==> T





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RX(4)

STAGE(1)

RGT D 100-44-7D PhCH<sub>2</sub>Cl, E 19232-39-4 Butanoic acid, 3-oxo-, ethyl ester, ion(1-), sodium (1:1)  
SOL 68-12-2 DMF  
CON 16 hours, 80 deg C

STAGE(2)

RGT F 7647-14-5 NaCl  
SOL 67-68-5 DMSO  
CON 48 hours, 140 deg C

STAGE(3)

RCT S 601-75-2  
RGT G 108-24-7 Ac<sub>2</sub>O, H 7664-93-9 H<sub>2</sub>SO<sub>4</sub>  
SOL 7732-18-5 Water

STAGE(4)

RCT B 70-11-1  
RGT I 127-09-3 AcONa, J 64-19-7 AcOH  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 1 hour, room temperature  
SUBSTAGE(2) 24 hours, room temperature

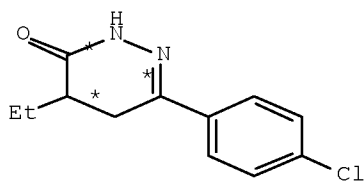
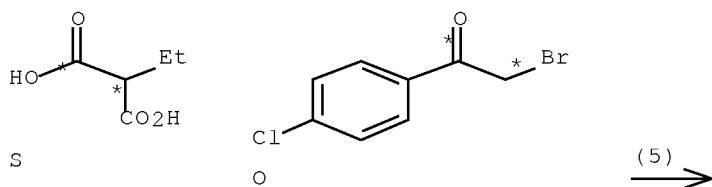
STAGE(5)

RGT K 302-01-2 N<sub>2</sub>H<sub>4</sub>  
SOL 7732-18-5 Water, 68-12-2 DMF  
CON 17 hours, room temperature

PRO T 24737-96-0

NTE solid-supported reagent, Merrifield resin used

RX(5) OF 9 S + O ==> U



U

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RX(5)

STAGE(1)

RGT D 100-44-7D PhCH<sub>2</sub>Cl, E 19232-39-4 Butanoic acid, 3-oxo-, ethyl ester, ion(1-), sodium (1:1)

SOL 68-12-2 DMF

CON 16 hours, 80 deg C

STAGE(2)

RGT F 7647-14-5 NaCl

SOL 67-68-5 DMSO

CON 48 hours, 140 deg C

STAGE(3)

RCT S 601-75-2

RGT G 108-24-7 Ac<sub>2</sub>O, H 7664-93-9 H<sub>2</sub>SO<sub>4</sub>

SOL 7732-18-5 Water

STAGE(4)

RCT O 536-38-9

RGT I 127-09-3 AcONa, J 64-19-7 AcOH

SOL 68-12-2 DMF

CON SUBSTAGE(1) 1 hour, room temperature

SUBSTAGE(2) 24 hours, room temperature

STAGE(5)

RGT K 302-01-2 N<sub>2</sub>H<sub>4</sub>

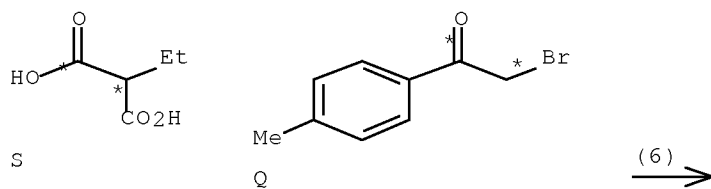
SOL 7732-18-5 Water, 68-12-2 DMF

CON 17 hours, room temperature

PRO U 746663-00-3

NTE solid-supported reagent, Merrifield resin used

RX(6) OF 9 S + Q ==> V



V

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RX(6)

STAGE(1)

RGT D 100-44-7D PhCH<sub>2</sub>Cl, E 19232-39-4 Butanoic acid, 3-oxo-, ethyl ester, ion(1-), sodium (1:1)  
SOL 68-12-2 DMF  
CON 16 hours, 80 deg C

STAGE(2)

RGT F 7647-14-5 NaCl  
SOL 67-68-5 DMSO  
CON 48 hours, 140 deg C

STAGE(3)

RCT S 601-75-2  
RGT G 108-24-7 Ac<sub>2</sub>O, H 7664-93-9 H<sub>2</sub>SO<sub>4</sub>  
SOL 7732-18-5 Water

STAGE(4)

RCT Q 619-41-0  
RGT I 127-09-3 AcONa, J 64-19-7 AcOH  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 1 hour, room temperature  
SUBSTAGE(2) 24 hours, room temperature

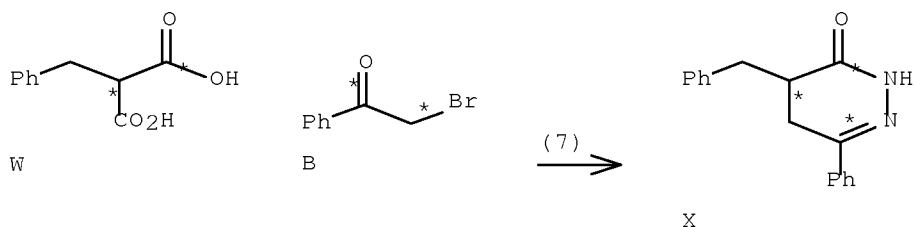
STAGE(5)

RGT K 302-01-2 N<sub>2</sub>H<sub>4</sub>  
SOL 7732-18-5 Water, 68-12-2 DMF  
CON 17 hours, room temperature

PRO V 24737-97-1

NTE solid-supported reagent, Merrifield resin used

RX(7) OF 9 W + B ==> X



RX(7)

STAGE(1)

RGT D 100-44-7D PhCH<sub>2</sub>Cl, E 19232-39-4 Butanoic acid, 3-oxo-, ethyl ester, ion(1-), sodium (1:1)  
SOL 68-12-2 DMF  
CON 16 hours, 80 deg C

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STAGE(2)

RGT F 7647-14-5 NaCl  
SOL 67-68-5 DMSO  
CON 48 hours, 140 deg C

STAGE(3)

RCT W 616-75-1  
RGT G 108-24-7 Ac2O, H 7664-93-9 H2SO4  
SOL 7732-18-5 Water

STAGE(4)

RCT B 70-11-1  
RGT I 127-09-3 AcONa, J 64-19-7 AcOH  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 1 hour, room temperature  
SUBSTAGE(2) 24 hours, room temperature

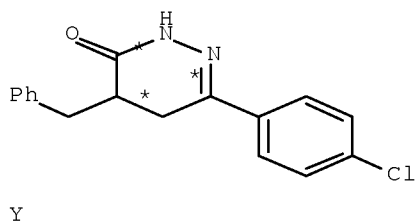
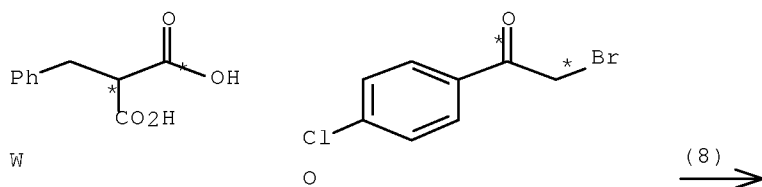
STAGE(5)

RGT K 302-01-2 N2H4  
SOL 7732-18-5 Water, 68-12-2 DMF  
CON 17 hours, room temperature

PRO X 202800-65-5

NTE solid-supported reagent, Merrifield resin used

RX(8) OF 9 W + O ==> Y



RX(8)

STAGE(1)

RGT D 100-44-7D PhCH2Cl, E 19232-39-4 Butanoic acid, 3-oxo-, ethyl ester, ion(1-), sodium (1:1)  
SOL 68-12-2 DMF

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CON 16 hours, 80 deg C

STAGE(2)

RGT F 7647-14-5 NaCl

SOL 67-68-5 DMSO

CON 48 hours, 140 deg C

STAGE(3)

RCT W 616-75-1

RGT G 108-24-7 Ac2O, H 7664-93-9 H2SO4

SOL 7732-18-5 Water

STAGE(4)

RCT O 536-38-9

RGT I 127-09-3 AcONa, J 64-19-7 AcOH

SOL 68-12-2 DMF

CON SUBSTAGE(1) 1 hour, room temperature

SUBSTAGE(2) 24 hours, room temperature

STAGE(5)

RGT K 302-01-2 N2H4

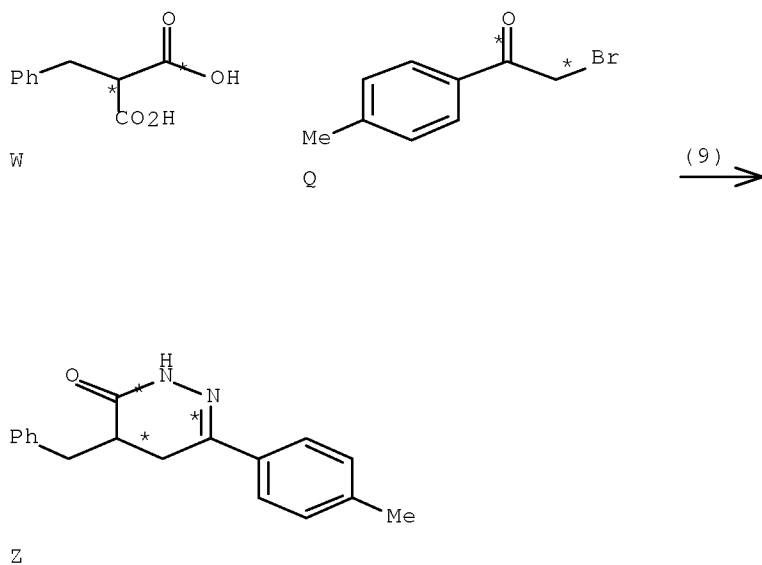
SOL 7732-18-5 Water, 68-12-2 DMF

CON 17 hours, room temperature

PRO Y 202800-75-7

NTE solid-supported reagent, Merrifield resin used

RX(9) OF 9 W + Q ==> Z



RX(9)

STAGE(1)

RGT D 100-44-7D PhCH2Cl, E 19232-39-4 Butanoic acid, 3-oxo-, ethyl ester, ion(1-), sodium (1:1)

SOL 68-12-2 DMF

CON 16 hours, 80 deg C

## STAGE(2)

RGT F 7647-14-5 NaCl  
SOL 67-68-5 DMSO  
CON 48 hours, 140 deg C

## STAGE(3)

RCT W 616-75-1  
RGT G 108-24-7 Ac2O, H 7664-93-9 H2SO4  
SOL 7732-18-5 Water

## STAGE(4)

RCT Q 619-41-0  
RGT I 127-09-3 AcONa, J 64-19-7 AcOH  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 1 hour, room temperature  
SUBSTAGE(2) 24 hours, room temperature

## STAGE(5)

RGT K 362-01-2 N2H4  
SOL 7732-18-5 Water, 68-12-2 DMF  
CON 17 hours, room temperature

PRO Z 746663-01-4

NTE solid-supported reagent, Merrifield resin used

L91 ANSWER 11 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 140:367760 CASREACT Full-text

TITLE: A New Route for Preparing Coordination Polymers from Hydrothermal Reactions Involving in Situ Ligand Synthesis

AUTHOR(S): Hu, Xi-Xue; Xu, Ji-Qing; Cheng, Peng; Chen, Xiao-Yan; Cui, Xiao-Bing; Song, Jiang-Feng; Yang, Guang-Di; Wang, Tie-Gang

CORPORATE SOURCE: College of Chemistry and State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, Jilin University, Changchun, 130023, Peop. Rep. China

SOURCE: Inorganic Chemistry (2004), 43(7), 2261-2266  
CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

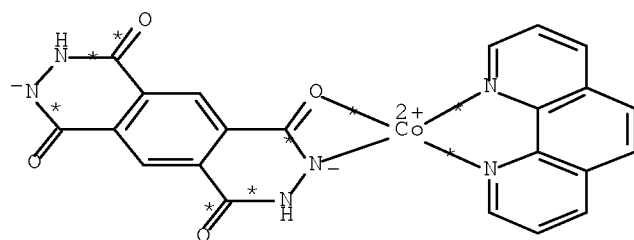
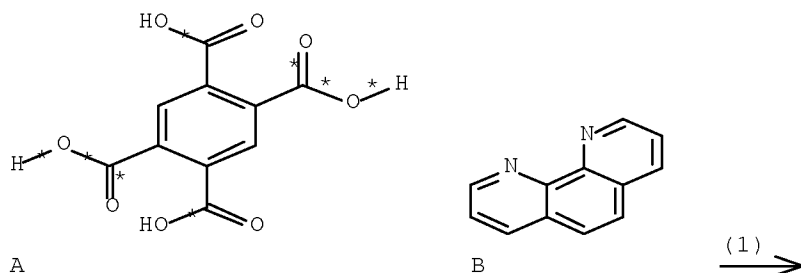
AB The coordination chemical of an inorg. cobalt salt and the organic ligands H4bbh (benzene-1,2,4,5-bihydrazide) and H3bcbh (benzene-4-carboxylate-1,2-bihydrazide) generated through the in situ hydrothermal acylate reaction of H4bta (benzene-1,2,4,5-tetracarboxylic acid) and H3btc (benzene-1,2,4-tricarboxylic acid) with hydrazine hydrate, resp., was studied. Three new coordination polymers were prepared and fully characterized by IR spectroscopy, elemental anal., and single-crystal x-ray diffraction. [Co( $\mu$ 3-H2bbh)(phen)]<sub>n</sub> (1, triclinic space group P $\bar{1}$  with *a* 9.762(4), *b* 10.169(4), *c* 11.143(4) Å,  $\alpha$  80.96(3),  $\beta$  64.49(3),  $\gamma$  71.88(3)°, *Z* = 2) was synthesized from the reaction of CoCl<sub>2</sub>·6H<sub>2</sub>O, H4bta (benzene-1,2,4,5-tetracarboxylic acid), N<sub>2</sub>H<sub>4</sub>·H<sub>2</sub>O, phen (1,10-phenanthroline) and H<sub>2</sub>O, and consists of 1-dimensional double-chains. [Co( $\mu$ 4-H2bbh)(H<sub>2</sub>O)<sub>2</sub>]<sub>n</sub> (2, monoclinic space group P2(1)/c with *a* 6.8687(5), *b* 7.5943(6), *c* 10.0401(6) Å,  $\beta$  95.250(4)°, *Z* = 2) was generated by the combination of CoCl<sub>2</sub>·6H<sub>2</sub>O, H4bta, N<sub>2</sub>H<sub>4</sub>·H<sub>2</sub>O, and H<sub>2</sub>O. It adopts a three-dimensional structural motif in the

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solid state with channels consisting of 20-numbered rings. [Co( $\mu^3$ -Hbcbh)(bpy)]<sub>n</sub> (3, monoclinic space group Cc with a 9.9464(13), b 23.685(5), c 7.9491(16) Å,  $\beta$  117.677(13)°, Z = 4) was obtained from the mixture of CoCl<sub>2</sub>·6H<sub>2</sub>O, N<sub>2</sub>H<sub>4</sub>·H<sub>2</sub>O, H<sub>3</sub>btc (benzene-1,2,4-tricarboxylic acid), bpy (2,2'-dipyridyl), and H<sub>2</sub>O, and features a two-dimensional plane. The results of magnetic research indicate that there exist antiferromagnetic interactions between Co centers in both compds. 1 and 2.

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 3 A + B ==> C

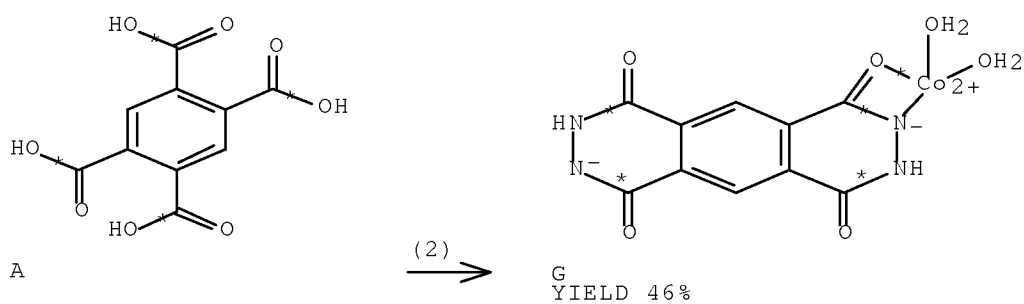


C  
YIELD 41%

RX(1) RCT A 89-05-4, B 66-71-7  
RGT D 7803-57-8 N<sub>2</sub>H<sub>4</sub>·H<sub>2</sub>O, E 7646-79-9 CoCl<sub>2</sub>  
PRO C 681439-74-7  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 4 days, 170 deg C  
SUBSTAGE(2) 170 deg C -> room temperature

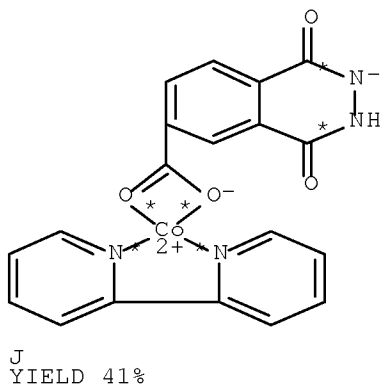
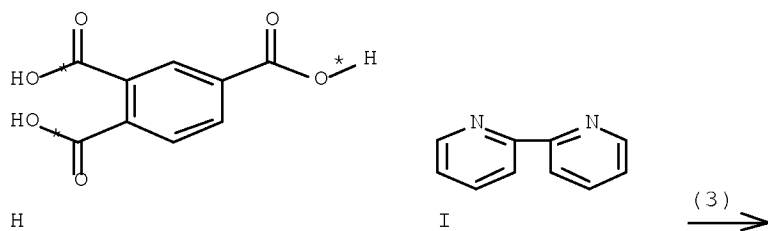
RX(2) OF 3 A ==> G

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RX(2)      RCT    A 89-05-4  
              RGT    D 7803-57-8 N2H4-H2O, E 7646-79-9 CoCl2, B  
                       66-71-7 1,10-Phenanthroline  
              PRO    G 681439-75-8  
              SOL    7732-18-5 Water  
              CON    SUBSTAGE(1) 4 days, 170 deg C  
                       SUBSTAGE(2) 170 deg C -> room temperature

RX(3) OF 3      H + I ==> J





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RX(3) RCT H 528-44-9, I 366-18-7  
 RGT D 7803-57-8 N2H4-H2O, E 7646-79-9 CoCl2  
 PRO J 681439-76-9  
 SOL 7732-18-5 Water  
 CON SUBSTAGE(1) 4 days, 170 deg C  
 SUBSTAGE(2) 170 deg C -> room temperature

L91 ANSWER 12 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 139:292230 CASREACT Full-text

TITLE: Synthesis and SAR of Thrombin Inhibitors Incorporating  
 a Novel 4-Amino-Morpholinone Scaffold: Analysis of  
 X-ray Crystal Structure of Enzyme Inhibitor Complex

AUTHOR(S): Nilsson, Jonas W.; Kvarnstrom, Ingemar; Musil,  
 Djordje; Nilsson, Ingemar; Samulesson, Bertil

CORPORATE SOURCE: Department of Chemistry, Linköping University,  
 Linköping, S-581 83, Swed.

SOURCE: Journal of Medicinal Chemistry (2003), 46(19),  
 3985-4001

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

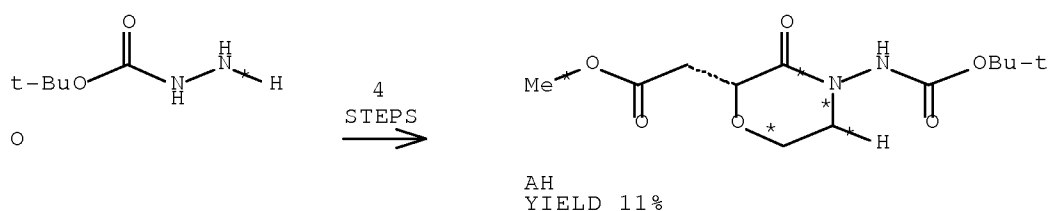
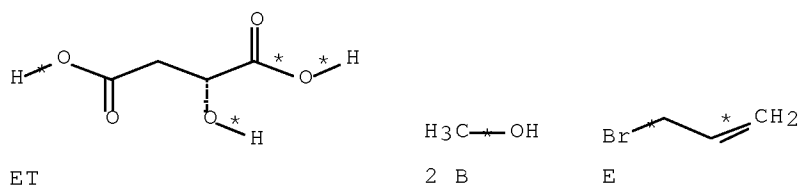
LANGUAGE: English

AB A 4-amino-2-carboxymethyl-3-morpholinone structural motif derived from malic acid has been used to mimic D-Phe-Pro in the thrombin inhibiting tripeptide D-Phe-Pro-Arg. The arginine in D-Phe-Pro-Arg was replaced by the more rigid P1 truncated p-amidinobenzylamine (Pab). These new thrombin inhibitors were used to probe the inhibitor binding site of  $\alpha$ -thrombin. The best candidate in this series of thrombin inhibitors exhibits an in vitro IC50 of 0.130  $\mu$ M. Interestingly, the stereochem. of the 4-amino-2-carboxymethyl-3-morpholinone motif is reversed for the most active compds. compared to that of a previously reported 2-carboxymethyl-3-morpholinone series. The X-ray crystal structure of the lead inhibitor cocrystd. with  $\alpha$ -thrombin is discussed.

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(349) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(10)

RX(349) ET + 2 B + E + O ==> AH



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RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2

CON room temperature

STAGE(2)

RCT E 106-95-6

RGT G 20667-12-3 Ag2O

SOL 108-88-3 PhMe

CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide

CAT 20816-12-0 OsO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

PRO ES 609847-51-0

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C

SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0

RGT R 1333-74-0 H2

PRO AG 609847-50-9

CAT 7440-05-3 Pd

SOL 109-99-9 THF

CON 18 hours, room temperature

RX(10) RCT AG 609847-50-9

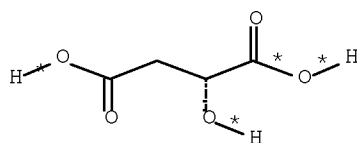
PRO AH 609846-38-0

SOL 108-88-3 PhMe

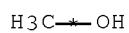
CON 3 days, reflux

RX(350) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97)

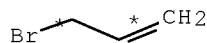
RX(350) ET + 2 B + E + O ==> AD



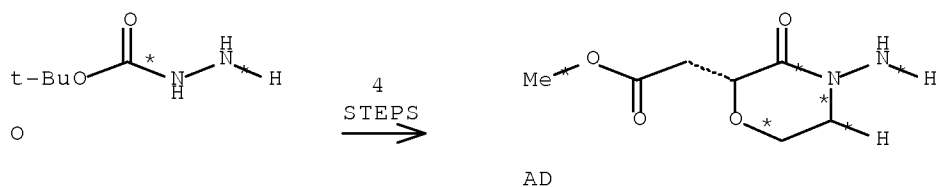
ET



2 B



E



RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl<sub>2</sub>

CON room temperature

STAGE(2)

RCT E 106-95-6

RGT G 20667-12-3 Ag<sub>2</sub>O

SOL 108-88-3 PhMe

CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide

CAT 20816-12-0 OsO<sub>4</sub>

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO<sub>4</sub>

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

PRO ES 609847-51-0

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C

SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0

RGT R 1333-74-0 H<sub>2</sub>

PRO AG 609847-50-9

CAT 7440-05-3 Pd

SOL 109-99-9 THF

CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9

PRO AD 609847-52-1

SOL 7732-18-5 Water

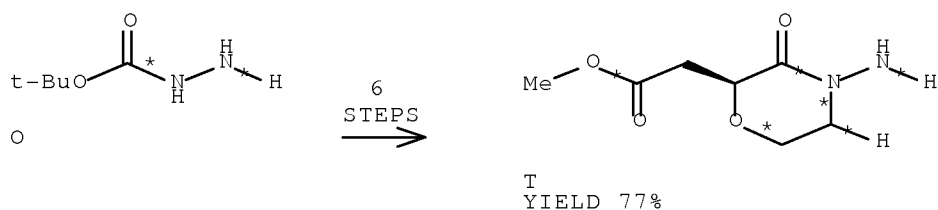
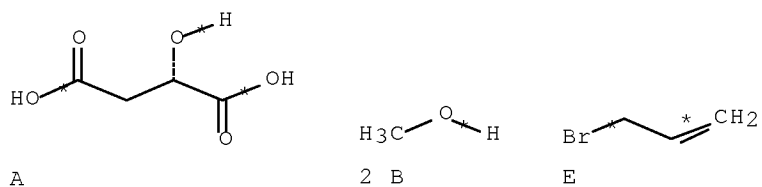
CON 7 hours, 60 deg C

NTE key intermediate

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RX(379) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6)

RX(379) A + 2 B + E + O ==> T



RX(1) RCT A 97-67-6, B 67-56-1  
 RGT D 7719-09-7 SOCl2  
 PRO C 617-55-0  
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
 RGT G 20667-12-3 Ag2O  
 PRO F 297749-53-2  
 SOL 108-88-3 PhMe  
 CON room temperature  
 NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)

RGT J 7529-22-8 Me-morpholineoxide  
 CAT 20816-12-0 OsO4  
 SOL 7732-18-5 Water, 109-99-9 THF  
 CON room temperature

STAGE(2)

RGT K 7790-28-5 NaIO4  
 SOL 7732-18-5 Water, 109-99-9 THF  
 CON room temperature

PRO I 441764-54-1

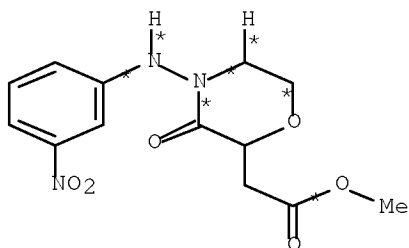
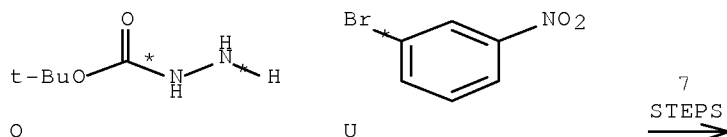
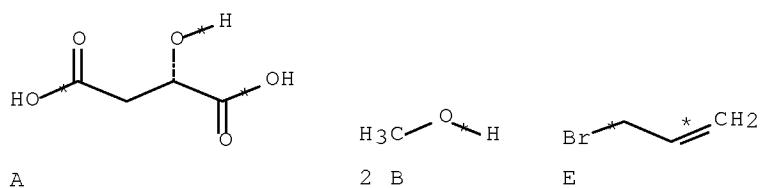
RX(4) RCT I 441764-54-1, O 870-46-2  
 PRO P 609846-32-4  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature -> 65 deg C  
 SUBSTAGE(2) overnight, 65 deg C

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RX(5) RCT P 609846-32-4  
 RGT R 1333-74-0 H2  
 PRO Q 609846-33-5  
 CAT 7440-05-3 Pd  
 SOL 109-99-9 THF  
 CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
 PRO T 609846-34-6  
 SOL 7732-18-5 Water  
 CON 7 hours, 60 deg C  
 NTE key intermediate

RX(426) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(7)  
 RX(426) A + 2 B + E + O + U ==> V



V  
 YIELD 33%

RX(1) RCT A 97-67-6, B 67-56-1  
 RGT D 7719-09-7 SOCl2

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```
PRO  C 617-55-0
CON  room temperature

RX(2)  RCT  C 617-55-0, E 106-95-6
      RGT  G 20667-12-3 Ag2O
      PRO  F 297749-53-2
      SOL  108-88-3 PhMe
      CON  room temperature
      NTE  other product also detected

RX(3)  RCT  F 297749-53-2

      STAGE(1)
      RGT  J 7529-22-8 Me-morpholineoxide
      CAT  20816-12-0 OsO4
      SOL  7732-18-5 Water, 109-99-9 THF
      CON  room temperature

      STAGE(2)
      RGT  K 7790-28-5 NaIO4
      SOL  7732-18-5 Water, 109-99-9 THF
      CON  room temperature

PRO  I 441764-54-1

RX(4)  RCT  I 441764-54-1, O 870-46-2
      PRO  P 609846-32-4
      SOL  108-88-3 PhMe
      CON  SUBSTAGE(1) room temperature -> 65 deg C
      SUBSTAGE(2) overnight, 65 deg C

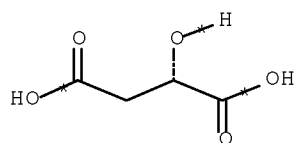
RX(5)  RCT  P 609846-32-4
      RGT  R 1333-74-0 H2
      PRO  Q 609846-33-5
      CAT  7440-05-3 Pd
      SOL  109-99-9 THF
      CON  18 hours, room temperature

RX(6)  RCT  Q 609846-33-5
      PRO  T 609846-34-6
      SOL  7732-18-5 Water
      CON  7 hours, 60 deg C
      NTE  key intermediate

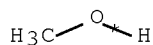
RX(7)  RCT  T 609846-34-6, U 585-79-5
      RGT  W 534-17-8 Cs2CO3
      PRO  V 609846-35-7
      CAT  161265-03-8 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-
      diyl)bis[1,1-diphenyl-, 3375-31-3 Pd(OAc)2
      SOL  108-88-3 PhMe
      CON  SUBSTAGE(1) room temperature
      SUBSTAGE(2) room temperature -> 95 deg C
      SUBSTAGE(3) 19 hours, 95 deg C

RX(427) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(8)
RX(427)  2 A + 4 B + 2 E + 2 O + 3 Z ==>
      AA + AB
```

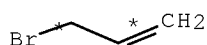
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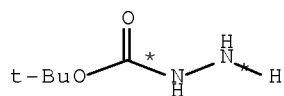
2 A



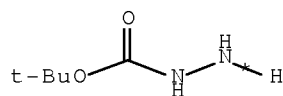
4 B



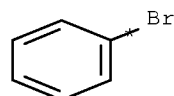
2 E



O

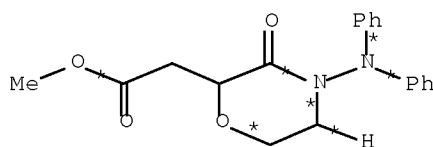


O

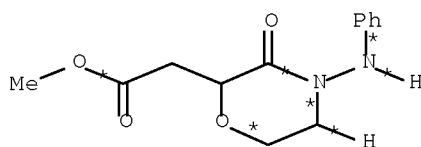


3 Z

7  
STEPS  
→



AA  
YIELD 58%



AB  
YIELD 58%

RX(1) RCT A 97-67-6, B 67-56-1  
RGT D 7719-09-7 SOCl2  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)

RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

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PRO I 441764-54-1

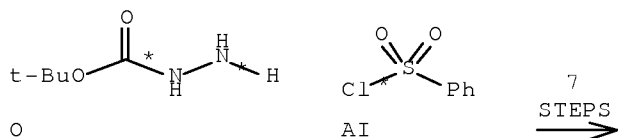
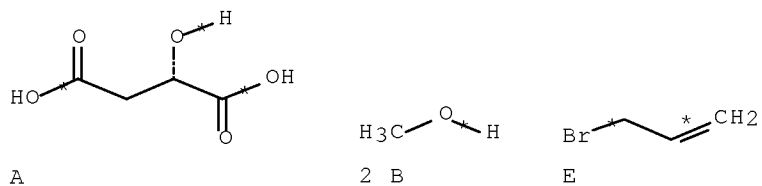
RX(4) RCT I 441764-54-1, O 870-46-2  
 PRO P 609846-32-4  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature -> 65 deg C  
 SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
 RGT R 1333-74-0 H2  
 PRO Q 609846-33-5  
 CAT 7440-05-3 Pd  
 SOL 109-99-9 THF  
 CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
 PRO T 609846-34-6  
 SOL 7732-18-5 Water  
 CON 7 hours, 60 deg C  
 NTE key intermediate

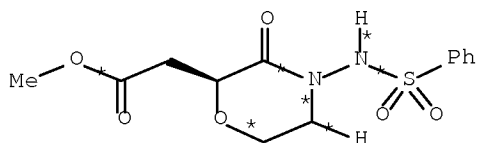
RX(8) RCT T 609846-34-6, Z 108-86-1  
 RGT W 534-17-8 Cs2CO3  
 PRO AA 609846-36-8, AB 609847-53-2  
 CAT 161265-03-8 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-diyl)bis[1,1-diphenyl-, 3375-31-3 Pd(OAc)2  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) room temperature -> 95 deg C  
 SUBSTAGE(3) 19 hours, 95 deg C

RX(428) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(12)  
 RX(428) A + 2 B + E + O + AI ==> AK





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AK  
YIELD 85%

RX(1) RCT A 97-67-6, B 67-56-1  
RGT D 7719-09-7 SOCl2  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

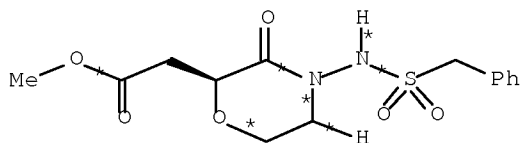
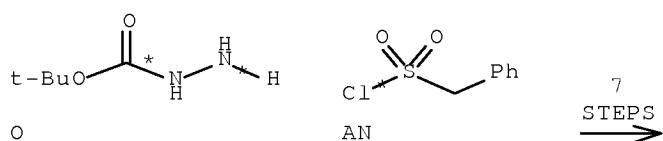
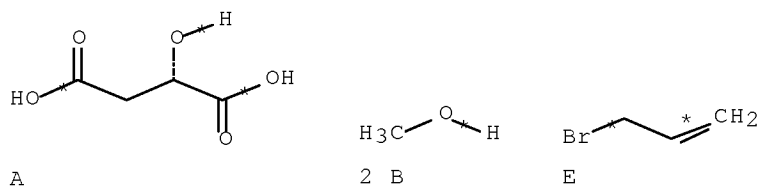
RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(12) RCT T 609846-34-6, AI 98-09-9

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PRO AK 609846-40-4  
 SOL 110-86-1 Pyridine  
 CON 20 hours, room temperature

RX(429) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(15)  
 RX(429) A + 2 B + E + O + AN ==> AP



AP  
 YIELD 39%

RX(1) RCT A 97-57-6, B 67-56-1  
 RGT D 7719-09-7 SOCl2  
 PRO C 617-55-0  
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
 RGT G 20667-12-3 Ag2O  
 PRO F 297749-53-2  
 SOL 108-88-3 PhMe  
 CON room temperature  
 NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)

RGT J 7529-22-8 Me-morpholineoxide  
 CAT 20816-12-0 OsO4

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SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)

RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

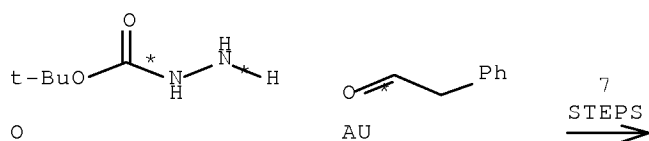
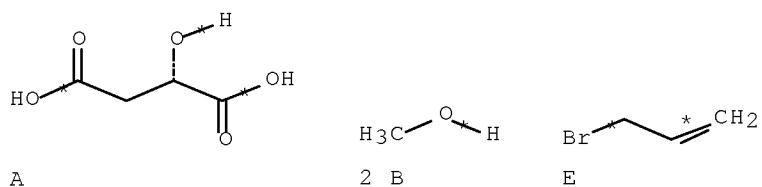
RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

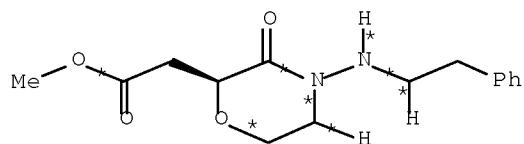
RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(15) RCT T 609846-34-6, AN 1939-99-7  
PRO AP 609846-43-7  
SOL 110-86-1 Pyridine  
CON SUBSTAGE(1) 24 hours, room temperature  
SUBSTAGE(2) room temperature -> 35 deg C  
SUBSTAGE(3) 3 days, 35 deg C

RX(430) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(19)  
RX(430) A + 2 B + E + O + AU ==> AW



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AW  
YIELD 63%

RX(1) RCT A 97-67-6, B 67-56-1  
RGT D 7719-09-7 SOCl<sub>2</sub>  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag<sub>2</sub>O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K 7790-28-5 NaIO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 370-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H<sub>2</sub>  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C

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NTE key intermediate

RX(19) RCT T 609846-34-6, AU 122-78-1

STAGE(1)

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) overnight, 60 deg C

STAGE(2)

RGT R 1333-74-0 H2

CAT 7440-05-3 Pd

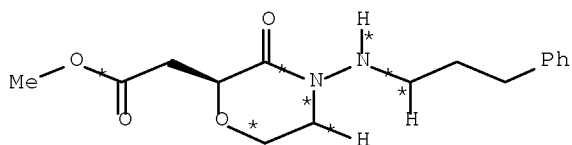
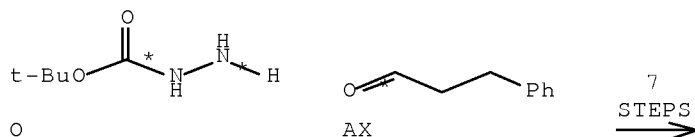
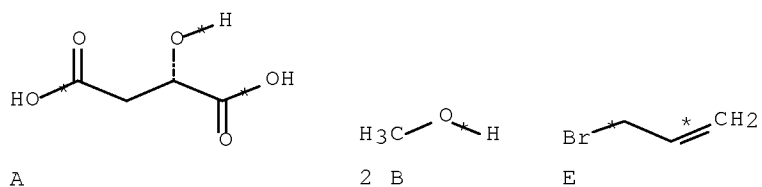
SOL 109-99-9 THF

CON 2 hours, room temperature

PRO AW 609846-47-1

RX(431) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(21)

RX(431) A + 2 B + E + O + AX ==> BA



BA  
YIELD 85%

RX(1) RCT A 97-67-6, B 67-56-1

RGT D 7719-09-7 SOCl2

PRO C 617-55-0

CON room temperature

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RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(21) RCT T 609846-34-6, AX 104-53-0

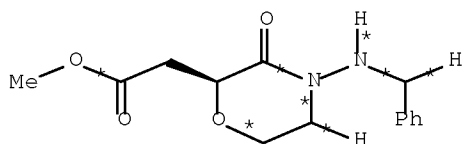
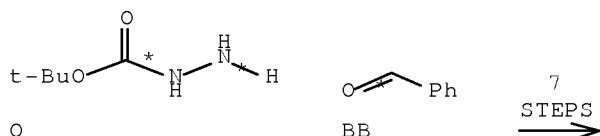
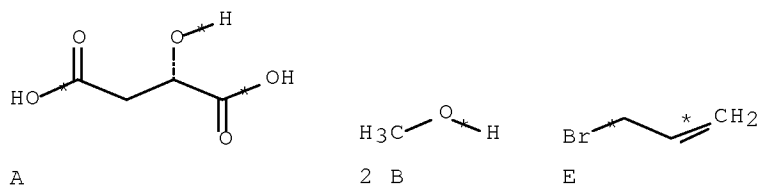
STAGE(1)  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) 5 hours, 70 deg C

STAGE(2)  
RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 3 hours, room temperature

PRO BA 609846-50-6

RX(432) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(23)  
RX(432) A + 2 B + E + O + BB ==> EE

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BE  
YIELD 56%

RX(1)      RCT    A 97-67-6, B 67-56-1  
               RGT    D 7719-09-7 SOCl2  
               PRO    C 617-55-0  
               CON    room temperature  
  
 RX(2)      RCT    C 617-55-0, E 106-95-6  
               RGT    G 20667-12-3 Ag2O  
               PRO    F 297749-53-2  
               SOL    108-88-3 PhMe  
               CON    room temperature  
               NTE    other product also detected  
  
 RX(3)      RCT    F 297749-53-2

STAGE(1)  
               RGT    J 7529-22-8 Me-morpholineoxide  
               CAT    20816-12-0 OsO4  
               SOL    7732-18-5 Water, 109-99-9 THF  
               CON    room temperature

STAGE(2)  
               RGT    K 7790-28-5 NaIO4  
               SOL    7732-18-5 Water, 109-99-9 THF  
               CON    room temperature

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PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(23) RCT T 609846-34-6, BB 100-52-7

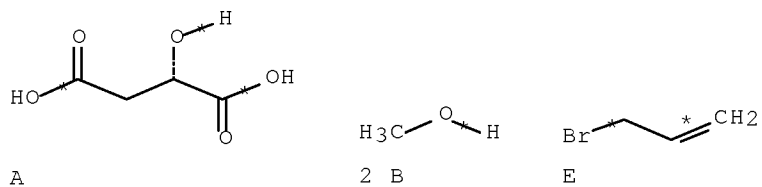
STAGE(1)  
RGT BD 1125-88-8 PhCH(OMe)2  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 80 deg C  
SUBSTAGE(2) 2 days, 80 deg C

STAGE(2)  
RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 5 minutes, room temperature

PRO BE 609846-52-8

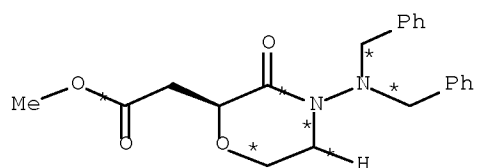
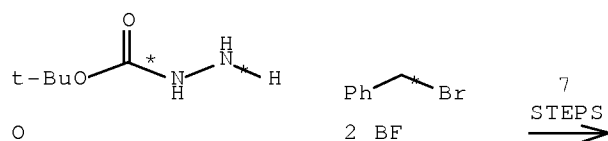
RX(433) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(24)

RX(433) A + 2 B + E + O + 2 BF ==> EG





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BG  
YIELD 60%

RX(1) RCT A 97-67-6, B 67-56-1  
 RGT D 7719-09-7 SOCl<sub>2</sub>  
 PRO C 617-55-0  
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
 RGT G 20667-12-3 Ag<sub>2</sub>O  
 PRO F 297749-53-2  
 SOL 108-88-3 PhMe  
 CON room temperature  
 NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
 RGT J 7529-22-8 Me-morpholineoxide  
 CAT 20816-12-0 OsO<sub>4</sub>  
 SOL 7732-18-5 Water, 109-99-9 THF  
 CON room temperature

STAGE(2)  
 RGT K 7790-28-5 NaIO<sub>4</sub>  
 SOL 7732-18-5 Water, 109-99-9 THF  
 CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
 PRO P 609846-32-4  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature -> 65 deg C  
 SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
 RGT R 1333-74-0 H<sub>2</sub>  
 PRO Q 609846-33-5

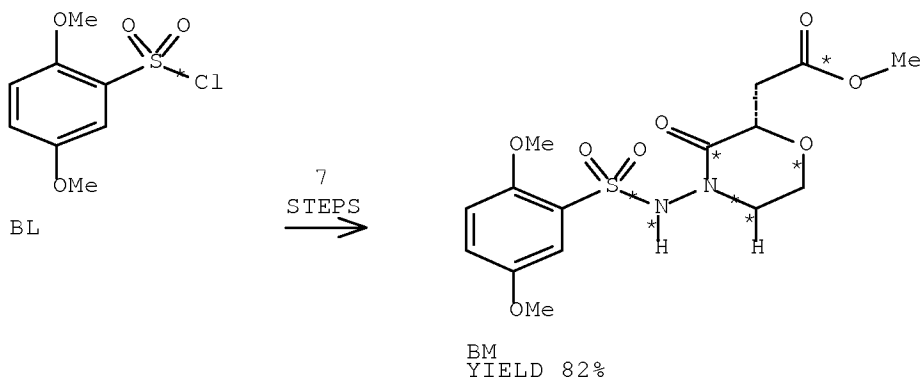
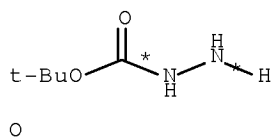
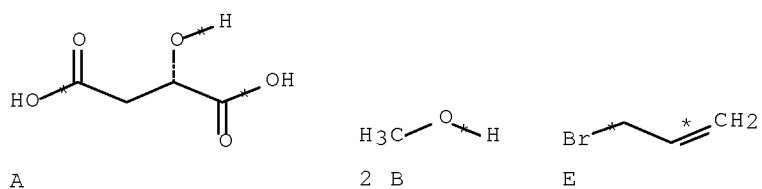
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CAT 7440-05-3 Pd  
 SOL 109-99-9 THF  
 CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
 PRO T 609846-34-6  
 SOL 7732-18-5 Water  
 CON 7 hours, 60 deg C  
 NTE key intermediate

RX(24) RCT T 609846-34-6, BF 100-39-0  
 RGT BH 7087-68-5 EtN(Pr-i)2, BI 144-55-8 NaHCO3  
 PRO BG 609846-53-9  
 CAT 10377-51-2 LiI  
 SOL 68-12-2 DMF  
 CON SUBSTAGE(1) room temperature -> 50 deg C  
 SUBSTAGE(2) 7 hours, 50 deg C

RX(434) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(25)  
 RX(434) A + 2 B + E + O + BL ==> BM



RX(1) RCT A ~~97-67-6~~, B 67-56-1  
 RGT D 7719-09-7 SOCl<sub>2</sub>  
 PRO C 617-55-0  
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
 RGT G 20667-12-3 Ag<sub>2</sub>O  
 PRO F 297749-53-2  
 SOL 108-88-3 PhMe  
 CON room temperature  
 NTE other product also detected

RX(3) RCT F 297749-53-2  
  
 STAGE(1)  
 RGT J 7529-22-8 Me-morpholineoxide  
 CAT 20816-12-0 OsO<sub>4</sub>  
 SOL 7732-18-5 Water, 109-99-9 THF  
 CON room temperature  
  
 STAGE(2)  
 RGT K ~~7790-28-5~~ NaIO<sub>4</sub>  
 SOL 7732-18-5 Water, 109-99-9 THF  
 CON room temperature  
  
 PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O ~~870-46-2~~  
 PRO P 609846-32-4  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature -> 65 deg C  
 SUBSTAGE(2) overnight, 65 deg C

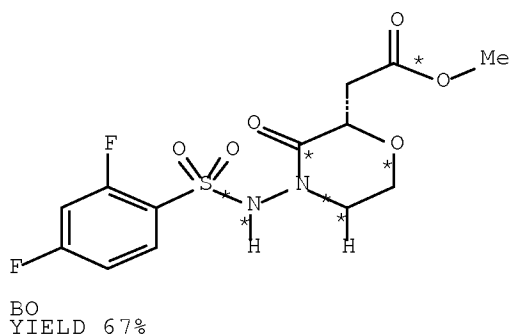
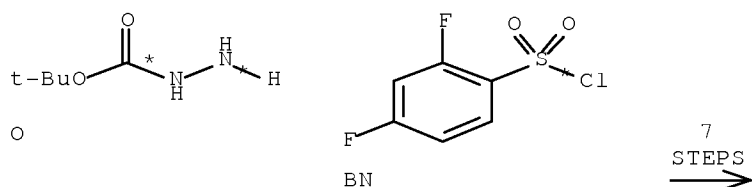
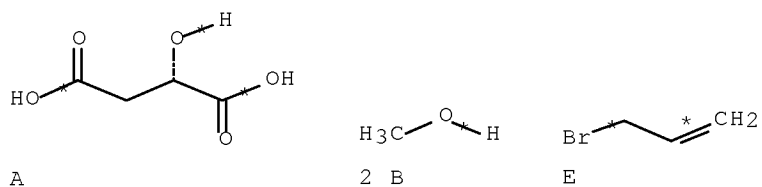
RX(5) RCT P 609846-32-4  
 RGT R 1333-74-0 H<sub>2</sub>  
 PRO Q 609846-33-5  
 CAT 7440-05-3 Pd  
 SOL 109-99-9 THF  
 CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
 PRO T 609846-34-6  
 SOL 7732-18-5 Water  
 CON 7 hours, 60 deg C  
 NTE key intermediate

RX(25) RCT T 609846-34-6, BL 1483-28-9  
 PRO ~~BM 609846-54-0~~  
 SOL 110-86-1 Pyridine  
 CON 24 hours, room temperature

RX(435) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(26)  
 RX(435) A + 2 B + E + O + BN ==> EO

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RX(1)      RCT    A 97-67-6, B 67-56-1  
               RGT    D 7719-09-7 SOCl2  
               PRO    C 617-55-0  
               CON    room temperature  
  
 RX(2)      RCT    C 617-55-0, E 106-95-6  
               RGT    G 20667-12-3 Ag2O  
               PRO    F 297749-53-2  
               SOL    108-88-3 PhMe  
               CON    room temperature  
               NTE    other product also detected  
  
 RX(3)      RCT    F 297749-53-2

STAGE(1)  
               RGT    J 7529-22-8 Me-morpholineoxide  
               CAT    20816-12-0 OsO4  
               SOL    7732-18-5 Water, 109-99-9 THF  
               CON    room temperature

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STAGE(2)

RGT K 7790-28-5 NaIO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2

PRO P 609846-32-4

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C

SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4

RGT R 1333-74-0 H2

PRO Q 609846-33-5

CAT 7440-05-3 Pd

SOL 109-99-9 THF

CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5

PRO T 609846-34-6

SOL 7732-18-5 Water

CON 7 hours, 60 deg C

NTE key intermediate

RX(26) RCT T 609846-34-6, BN 13918-92-8

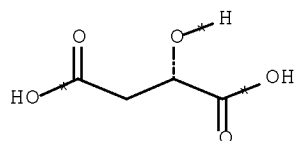
PRO BO 609846-55-1

SOL 110-86-1 Pyridine

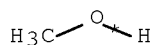
CON 24 hours, room temperature

RX(436) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(27)

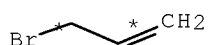
RX(436) A + 2 B + E + O + BP ==> BQ



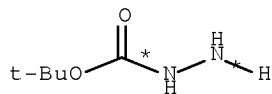
A



2 B

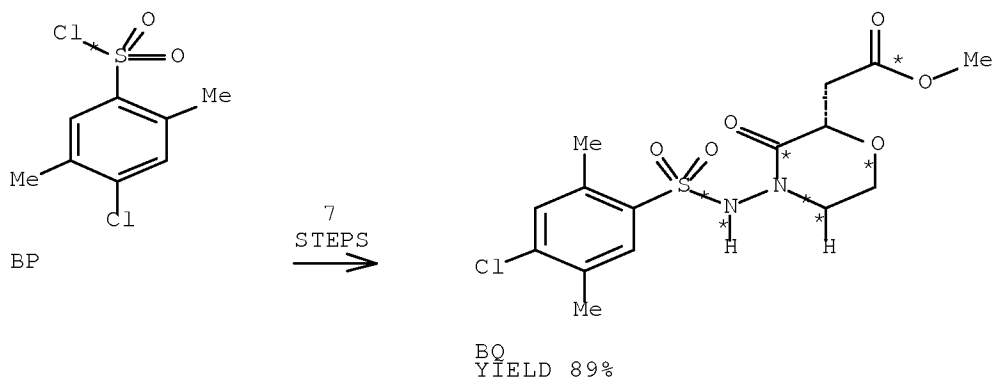


E



O

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RX(1) RCT A 97-67-6, B 67-56-1  
RGT D 7719-09-7 SOCl<sub>2</sub>  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag<sub>2</sub>O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K 7790-28-5 NaIO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H<sub>2</sub>  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

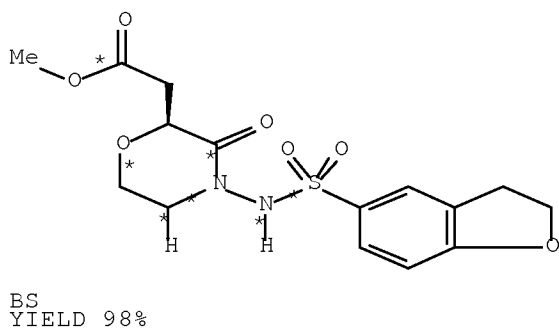
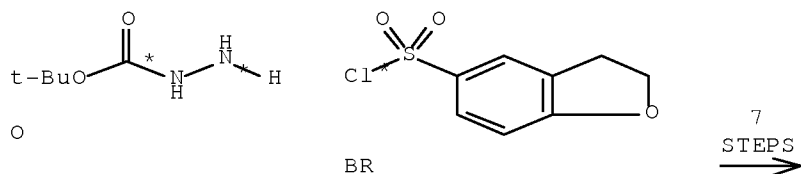
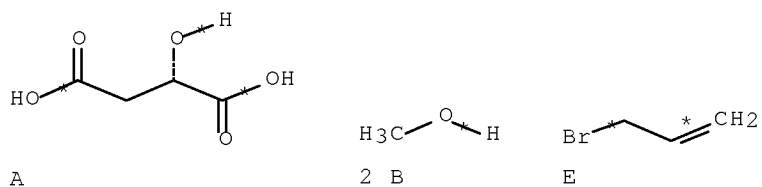
RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6

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SOL 7732-18-5 Water  
 CON 7 hours, 60 deg C  
 NTE key intermediate

RX(27) RCT T 609846-34-6, BP 88-49-3  
 PRO BQ 609846-56-2  
 SOL 110-86-1 Pyridine  
 CON 24 hours, room temperature

RX(437) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(28)  
 RX(437) A + 2 B + E + O + BR ==> BS



RX(1) RCT A 97-67-6, B 67-56-1  
 RGT D 7719-09-7 SOCl2  
 PRO C 617-55-0  
 CON room temperature

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RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

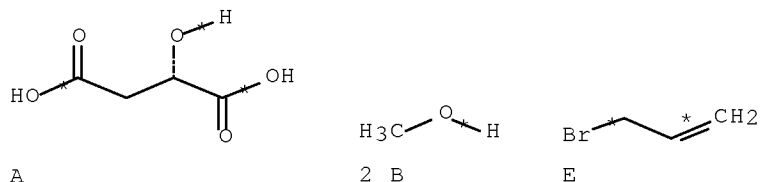
RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

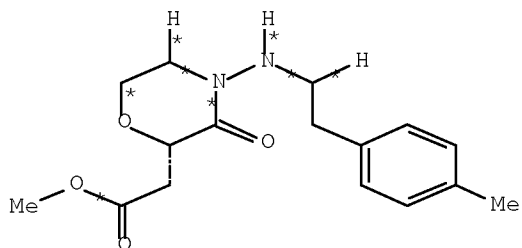
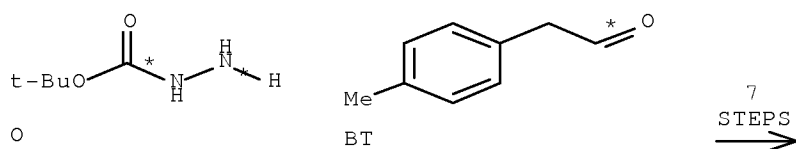
RX(28) RCT T 609846-34-6, BR 115010-11-2  
PRO BS 609846-57-3  
SOL 110-86-1 Pyridine  
CON 90 minutes, room temperature

RX(438) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(29)  
RX(438) A + 2 B + E + O + BT ==> EU





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BU  
YIELD 47%

RX(1) RCT A 97-67-6, B 67-56-1  
 RGT D 7719-09-7 SOCl<sub>2</sub>  
 PRO C 617-55-0  
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
 RGT G 20667-12-3 Ag<sub>2</sub>O  
 PRO F 297749-53-2  
 SOL 108-88-3 PhMe  
 CON room temperature  
 NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
 RGT J 7529-22-8 Me-morpholineoxide  
 CAT 20816-12-0 OsO<sub>4</sub>  
 SOL 7732-18-5 Water, 109-99-9 THF  
 CON room temperature

STAGE(2)  
 RGT K 7790-28-5 NaIO<sub>4</sub>  
 SOL 7732-18-5 Water, 109-99-9 THF  
 CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
 PRO P 609846-32-4  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature -> 65 deg C

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SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
 RGT R 1333-74-0 H2  
 PRO Q 609846-33-5  
 CAT 7440-05-3 Pd  
 SOL 109-99-9 THF  
 CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
 PRO T 609846-34-6  
 SOL 7732-18-5 Water  
 CON 7 hours, 60 deg C  
 NTE key intermediate

RX(29) RCT T 609846-34-6, BT 104-09-6

STAGE(1)

SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) overnight, 75 deg C

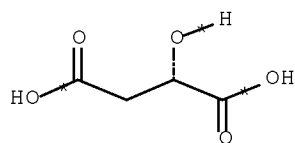
STAGE(2)

RGT R 1333-74-0 H2  
 CAT 7440-05-3 Pd  
 SOL 109-99-9 THF  
 CON 24 hours, room temperature

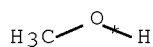
PRO BU 609846-58-4

RX(439) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(75)

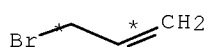
RX(439) A + 2 B + E + O + AI + CL + DM ==>  
 DU



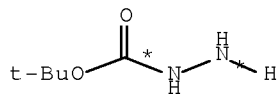
A



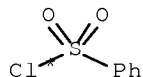
2 B



E

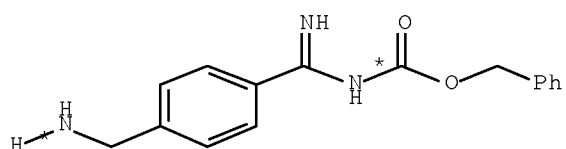


O



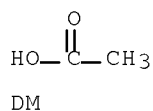
AI

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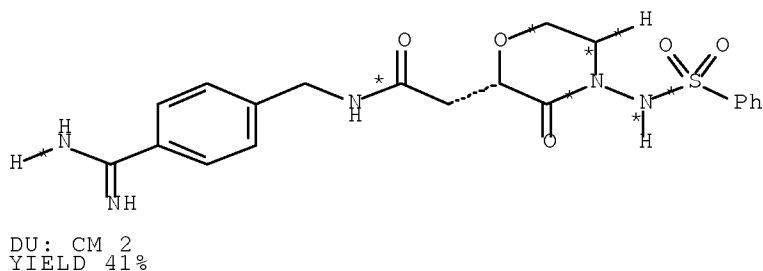
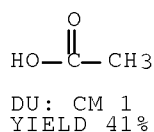


CL

● 2 HCl



7  
STEPS  
→



RX(1) RCT A 97-67-6, B 67-56-1  
RGT D 7719-09-7 SOCl2  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe

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CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(75) RCT T 609846-34-6, AI 98-09-9

STAGE(1)  
SOL 110-86-1 Pyridine  
CON 20 hours, room temperature

STAGE(2)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(3)  
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

STAGE(4)  
RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

STAGE(5)  
RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 7732-18-5 Water, 64-17-5 EtOH  
CON 1 hour, room temperature

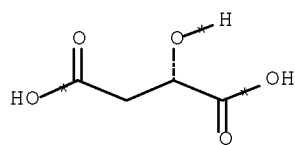
STAGE(6)  
RCT DM 64-19-7  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

PRO DU 609847-12-3

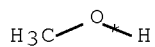
RX(440) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(78)

RX(440) A + 2 B + E + O + AN + CL + DM ==>  
DX

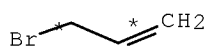
10/595943



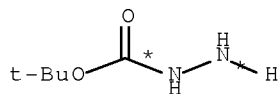
A



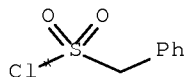
2 B



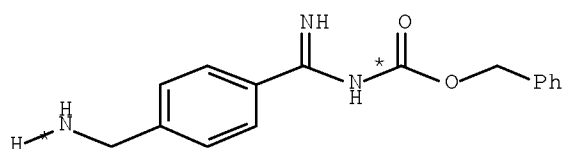
E



O

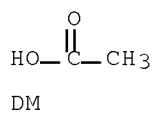


AN



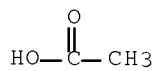
CL

● 2 HCl

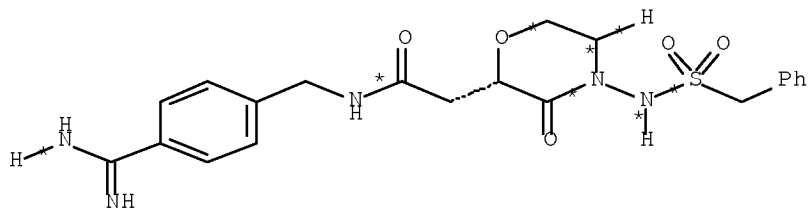


DM

7  
STEPS  
➔



DX: CM 1  
YIELD 8%



DX: CM 2  
YIELD 8%

RX(1) RCT A 97-67-6, B 67-56-1  
RGT D 7719-09-7 SOCl2  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6

10/595943

RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(78) RCT T 609846-34-6, AN 1939-99-7

STAGE(1)  
SOL 110-86-1 Pyridine  
CON SUBSTAGE(1) 24 hours, room temperature  
SUBSTAGE(2) room temperature -> 35 deg C  
SUBSTAGE(3) 3 days, 35 deg C

STAGE(2)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(3)  
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

STAGE(4)  
RCT CL 172348-75-3

10/595943

RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

STAGE(5)

RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 7732-18-5 Water, 64-17-5 EtOH  
CON 1 hour, room temperature

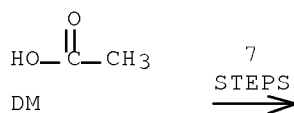
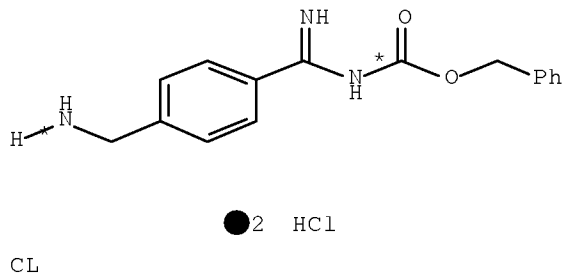
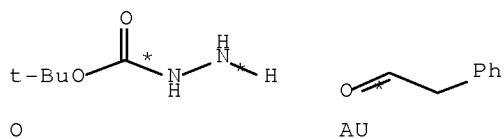
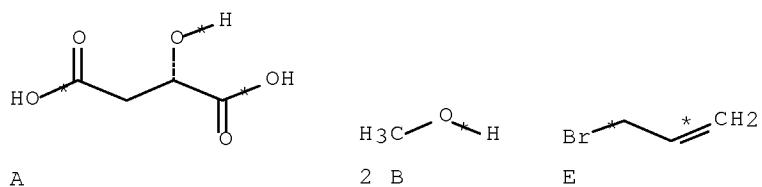
STAGE(6)

RCT DM 64-19-7  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

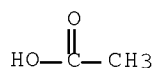
PRO DX 609847-18-9

RX(441) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(82)

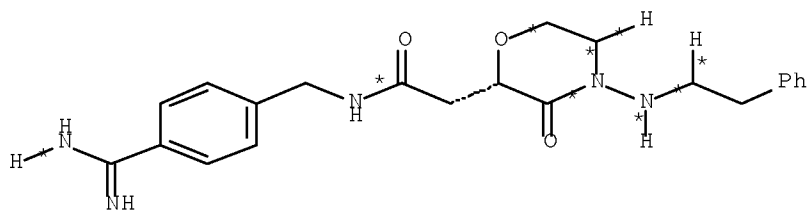
RX(441) A + 2 B + E + O + AU + CL + DM ==>  
EE



10/595943



EB: CM 1  
YIELD 51%



EB: CM 2  
YIELD 51%

RX(1) RCT A 97-67-6, B 67-56-1  
RGT D 7719-09-7 SOCl2  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6



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SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(82) RCT T 609846-34-6, AU 122-78-1

STAGE(1)

SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) overnight, 60 deg C

STAGE(2)

RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 2 hours, room temperature

STAGE(3)

RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(4)

RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

STAGE(5)

RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

STAGE(6)

RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 7732-18-5 Water, 64-17-5 EtOH  
CON 2 hours, room temperature

STAGE(7)

RCT DM 64-19-7  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

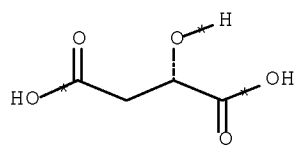
PRO EB 609847-26-9

RX(442) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(84)

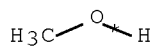
RX(442) A + 2 B + E + O + AX + CL + DM ==>

ED

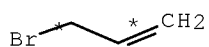
10/595943



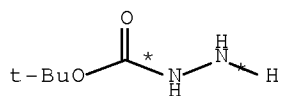
A



2 B



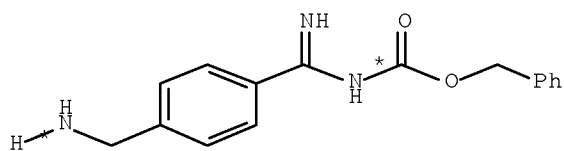
E



O

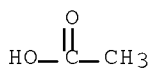


AX



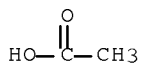
CL

2 HCl

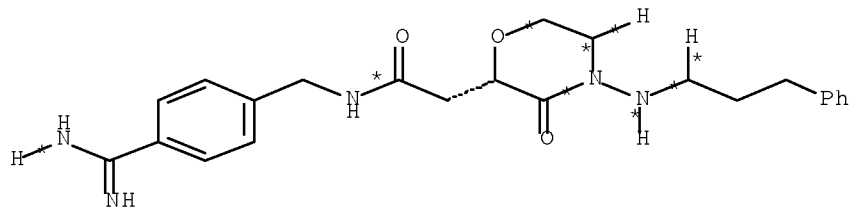


DM

7  
STEPS  
→



ED: CM 1  
YIELD 15%



ED: CM 2  
YIELD 15%

RX(1) RCT A ~~97-67-6~~, B 67-56-1  
RGT D 7719-09-7 SOCl<sub>2</sub>  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag<sub>2</sub>O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K ~~7790-28-5~~ NaIO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O ~~870-46-2~~  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H<sub>2</sub>  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(84) RCT T 609846-34-6, AX 104-53-0

STAGE(1)  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) 5 hours, 70 deg C

STAGE(2)  
RGT R 1333-74-0 H<sub>2</sub>  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 3 hours, room temperature

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STAGE(3)

RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(4)

RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

STAGE(5)

RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

STAGE(6)

RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 7732-18-5 Water, 64-17-5 EtOH  
CON 2 hours, room temperature

STAGE(7)

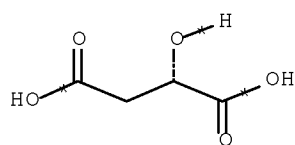
RCT DM 64-19-7  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

PRO ED 609847-30-5

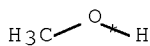
RX(443) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(88)

RX(443) A + 2 B + E + O + 2 BF + CL + DM

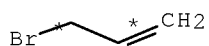
====> EL



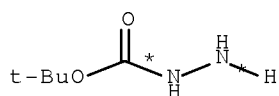
A



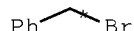
2 B



E

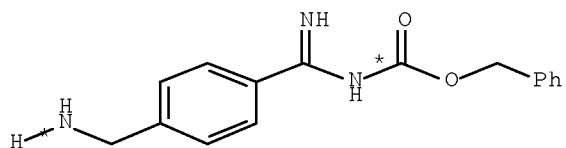


O

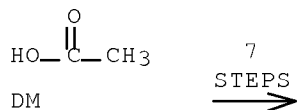


2 BF

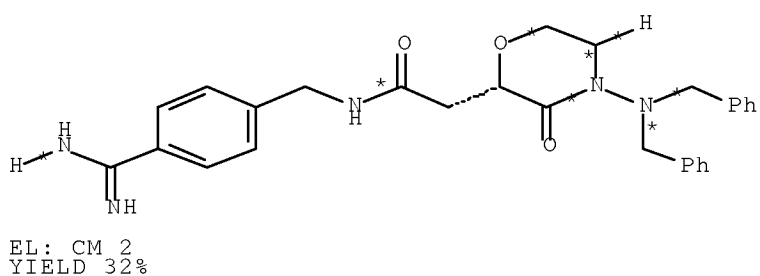
10/595943



CL  
● 2 HCl



HO-C(=O)-CH<sub>3</sub>  
EL: CM 1  
YIELD 32%



RX(1) RCT A 97-67-6, B 67-56-1  
RGT D 7719-09-7 SOCl<sub>2</sub>  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag<sub>2</sub>O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K 7790-28-5 NaIO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4

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SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(88) RCT T 609846-34-6, BF 100-39-0

STAGE(1)  
RGT BH 7087-68-5 EtN(Pr-i)2, BI 144-55-8 NaHCO3  
CAT 10377-51-2 LiI  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) room temperature -> 50 deg C  
SUBSTAGE(2) 7 hours, 50 deg C

STAGE(2)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(3)  
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

STAGE(4)  
RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

STAGE(5)  
RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 7732-18-5 Water, 64-17-5 EtOH  
CON 24 hours, room temperature

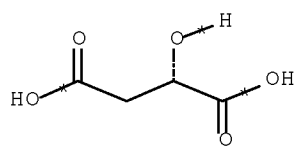
STAGE(6)  
RCT DM 64-19-7  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

PRO EL 609847-37-2

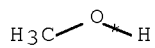
RX(444) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(89)  
RX(444) A + 2 B + E + O + BL + CL + DM ==>

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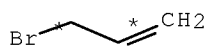
EM



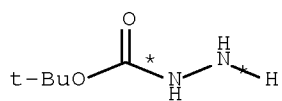
A



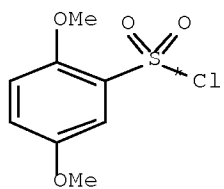
2 B



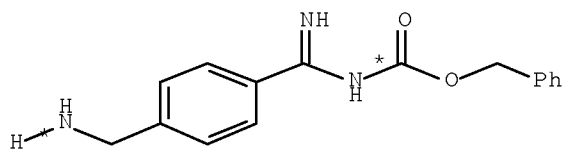
E



O

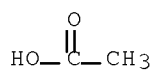


BL



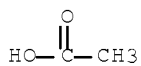
CL

● 2 HCl



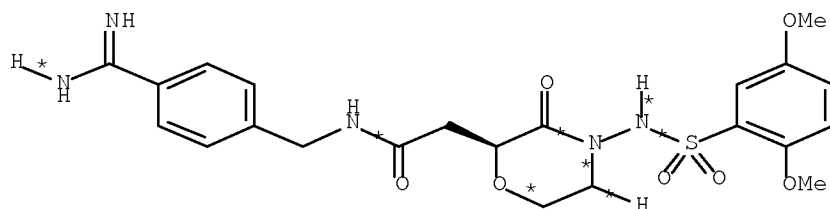
DM

7  
STEPS  
➔



EM: CM 1  
YIELD 49%

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EM: CM 2  
YIELD 49%

RX(1) RCT A 97-67-6, B 67-56-1  
RGT D 7719-09-7 SOCl2  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate



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RX(89) RCT T 609846-34-6, BL 1483-28-9

STAGE(1)

SOL 110-86-1 Pyridine  
CON 24 hours, room temperature

STAGE(2)

RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(3)

RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

STAGE(4)

RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

STAGE(5)

RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 7732-18-5 Water, 64-17-5 EtOH  
CON 24 minutes, room temperature

STAGE(6)

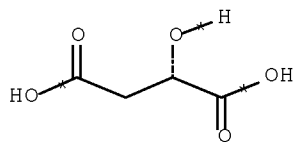
RCT DM 64-19-7  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

PRO EM 609847-39-4

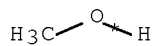
RX(445) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(90)

RX(445) A + 2 B + E + O + BN + CL + DM ==>

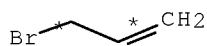
EN



A

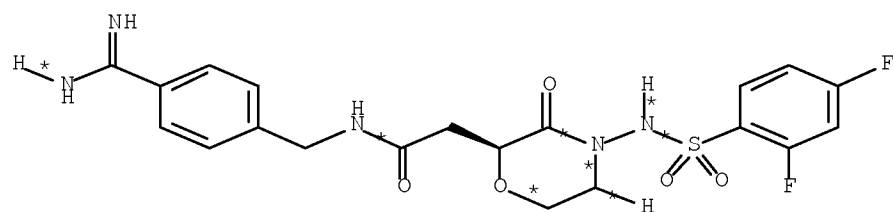
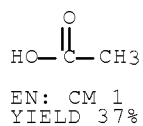
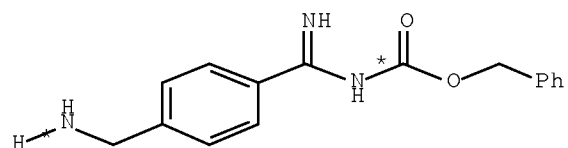
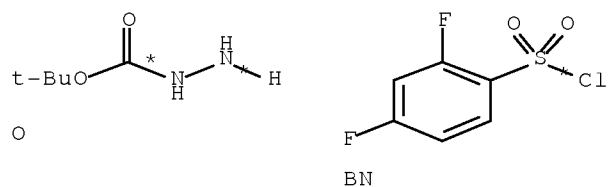


2 B



E

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EN: CM 2  
 YIELD 37%

RX(1) RCT A 97-67-6, B 67-56-1  
 RGT D 7719-09-7 SOCl<sub>2</sub>  
 PRO C 617-55-0  
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
 RGT G 20667-12-3 Ag<sub>2</sub>O  
 PRO F 297749-53-2

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SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K ~~7790-28-5~~ NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O ~~870-46-2~~  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(90) RCT T 609846-34-6, BN 13918-92-8

STAGE(1)  
SOL 110-86-1 Pyridine  
CON 24 hours, room temperature

STAGE(2)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(3)  
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

STAGE(4)  
RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF

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CON 100 minutes, room temperature

STAGE(5)

RGT R 1333-74-0 H2

CAT 7440-05-3 Pd

SOL 7732-18-5 Water, 64-17-5 EtOH

CON 24 minutes, room temperature

STAGE(6)

RCT DM 64-19-7

SOL 7732-18-5 Water, 67-56-1 MeOH

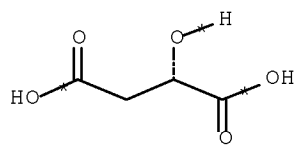
CON room temperature

PRO EN 609847-41-8

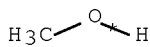
RX(446) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(91)

RX(446) 2 A + 4 B + 2 E + 2 O + 2 BP + 2 CL +

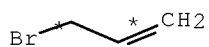
2 DM ==> EO + EP



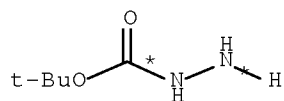
2 A



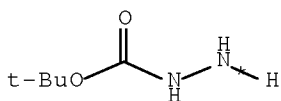
4 B



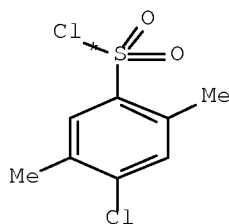
2 E



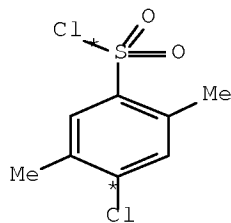
O



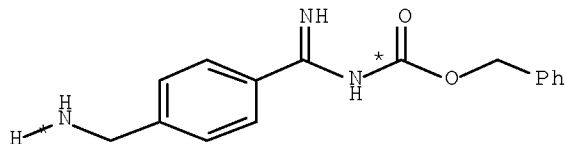
O



BP

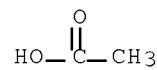


BP



2 CL

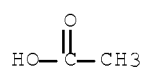
● 2 HCl



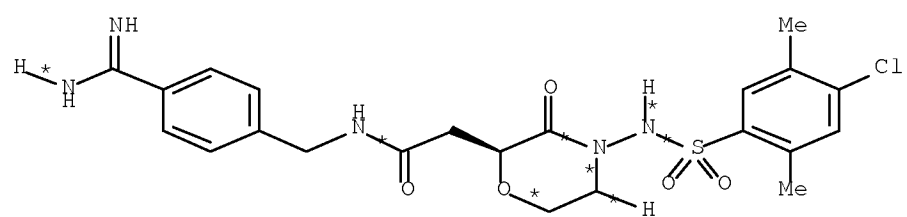
2 DM

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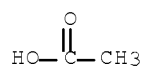
7  
STEPS  
→



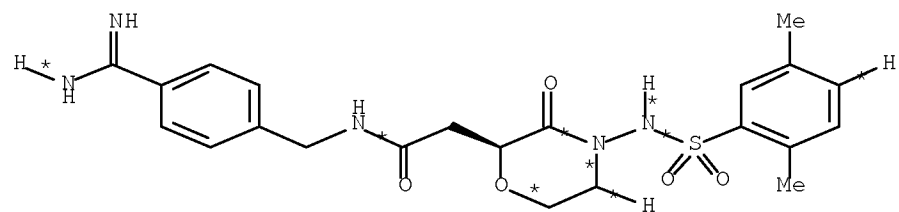
EO: CM 1  
YIELD 13%



EO: CM 2  
YIELD 13%



EP: CM 1  
YIELD 24%



EP: CM 2  
YIELD 24%

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RX(1) RCT A 97-57-6, B 67-56-1  
RGT D 7719-09-7 SOCl<sub>2</sub>  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag<sub>2</sub>O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K 7790-28-5 NaIO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H<sub>2</sub>  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(91) RCT T 609846-34-6, BP 88-49-3

STAGE(1)  
SOL 110-86-1 Pyridine  
CON 24 hours, room temperature

STAGE(2)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(3)  
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water

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CON room temperature

STAGE(4)

RCT CL 172348-75-3

RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2

SOL 68-12-2 DMF

CON 100 minutes, room temperature

STAGE(5)

RGT R 1333-74-0 H2

CAT 7440-05-3 Pd

SOL 7732-18-5 Water, 64-17-5 EtOH

CON 29 minutes, room temperature

STAGE(6)

RCT DM 64-19-7

SOL 7732-18-5 Water, 67-56-1 MeOH

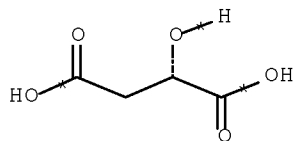
CON room temperature

PRO EO 609847-43-0, EP 609847-45-2

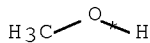
RX(447) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(92)

RX(447) A + 2 B + E + O + BR + CL + DM ==>

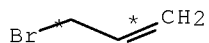
EQ



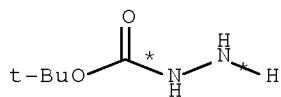
A



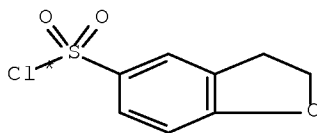
2 B



E

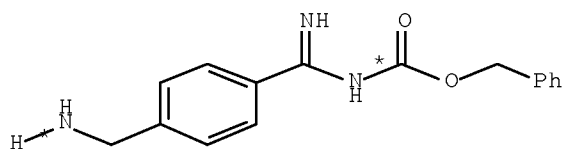


O



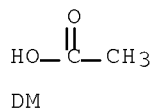
BR

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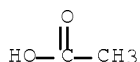


CL

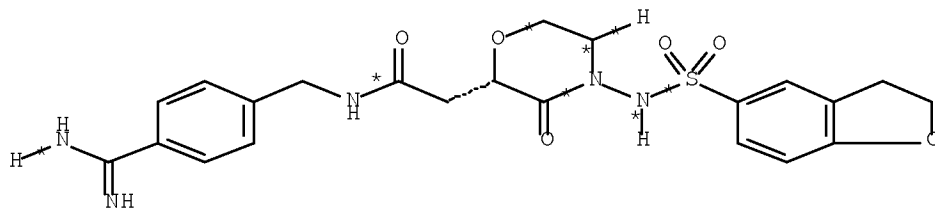
● 2 HCl



7  
STEPS  
→



EQ: CM 1  
YIELD 59%



EQ: CM 2  
YIELD 59%

RX(1) RCT A 97-67-6, B 67-56-1  
RGT D 7719-09-7 SOCl2  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature



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```
STAGE(2)
  RGT  K 7790-28-5 NaIO4
  SOL  7732-18-5 Water, 109-99-9 THF
  CON  room temperature

PRO   I 441764-54-1

RX(4)  RCT  I 441764-54-1, O 870-46-2
      PRO  P 609846-32-4
      SOL  108-88-3 PhMe
      CON  SUBSTAGE(1) room temperature -> 65 deg C
          SUBSTAGE(2) overnight, 65 deg C

RX(5)  RCT  P 609846-32-4
      RGT  R 1333-74-0 H2
      PRO  Q 609846-33-5
      CAT  7440-05-3 Pd
      SOL  109-99-9 THF
      CON  18 hours, room temperature

RX(6)  RCT  Q 609846-33-5
      PRO  T 609846-34-6
      SOL  7732-18-5 Water
      CON  7 hours, 60 deg C
      NTE  key intermediate

RX(92) RCT  T 609846-34-6, BR 115010-11-2

STAGE(1)
  SOL  110-86-1 Pyridine
  CON  90 minutes, room temperature

STAGE(2)
  RGT  BW 1310-65-2 LiOH
  SOL  7732-18-5 Water, 67-56-1 MeOH
  CON  room temperature

STAGE(3)
  RGT  BX 7647-01-0 HCl
  SOL  7732-18-5 Water
  CON  room temperature

STAGE(4)
  RCT  CL 172348-75-3
  RGT  CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
      1-[bis(dimethylamino)methylene]-, 3-oxide,
      hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
  SOL  68-12-2 DMF
  CON  100 minutes, room temperature

STAGE(5)
  RGT  R 1333-74-0 H2
  CAT  7440-05-3 Pd
  SOL  7732-18-5 Water, 64-17-5 EtOH, 109-99-9 THF
  CON  1 hour, room temperature

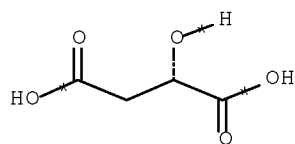
STAGE(6)
  RCT  DM 64-19-7
  SOL  7732-18-5 Water, 67-56-1 MeOH
  CON  room temperature
```

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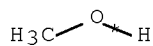
PRO EQ 609847-47-4

RX(448) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(93)

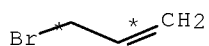
RX(448) A + 2 B + E + O + BT + CL + DM ==>  
ER



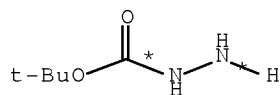
A



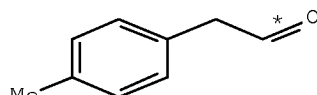
2 B



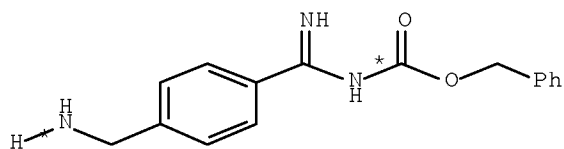
E



O

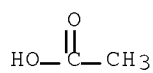


BT



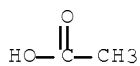
CL

● 2 HCl



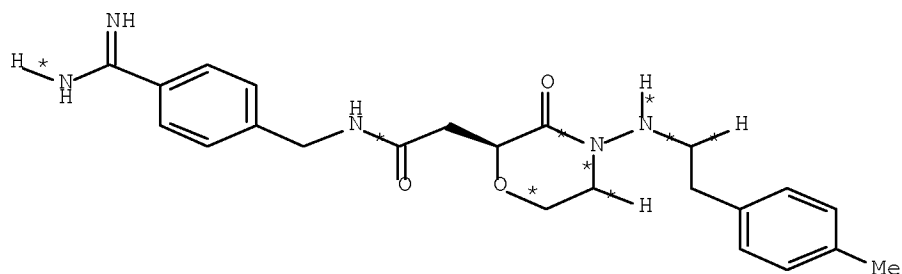
DM

7  
STEPS  
→



ER: CM 1  
YIELD 32%

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ER: CM 2  
YIELD 32%

RX(1) RCT A 97-67-6, B 67-56-1  
RGT D 7719-09-7 SOCl2  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water

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CON 7 hours, 60 deg C  
NTE key intermediate

RX(93) RCT T 609846-34-6, BT 104-09-6

STAGE(1)

SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) overnight, 75 deg C

STAGE(2)

RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 24 hours, room temperature

STAGE(3)

RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(4)

RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

STAGE(5)

RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

STAGE(6)

RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 7732-18-5 Water, 64-17-5 EtOH  
CON 25 minutes, room temperature

STAGE(7)

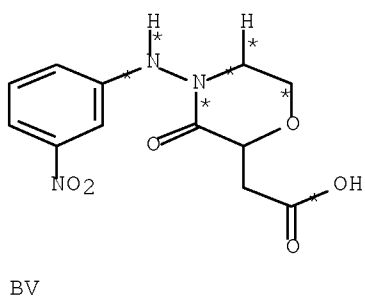
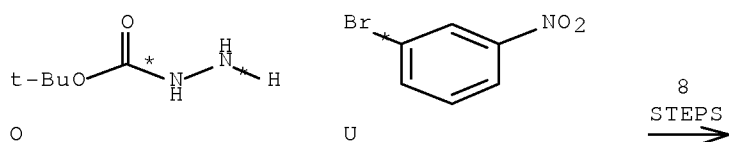
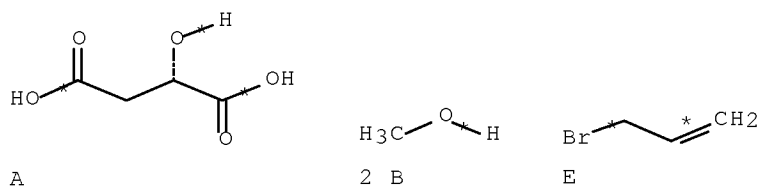
RCT DM 64-19-7  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

PRO ER 609847-49-6

RX(503) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(7),  
RX(30)

RX(503) A + 2 B + E + O + U ==> EV

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RX(1)      RCT    A 97-67-6, B 67-56-1  
               RGT    D 7719-09-7 SOCl2  
               PRO    C 617-55-0  
               CON    room temperature  
  
 RX(2)      RCT    C 617-55-0, E 106-95-6  
               RGT    G 20667-12-3 Ag2O  
               PRO    F 297749-53-2  
               SOL    108-88-3 PhMe  
               CON    room temperature  
               NTE    other product also detected  
  
 RX(3)      RCT    F 297749-53-2

STAGE(1)  
               RGT    J 7529-22-8 Me-morpholineoxide  
               CAT    20816-12-0 OsO4  
               SOL    7732-18-5 Water, 109-99-9 THF  
               CON    room temperature

STAGE(2)

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RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(7) RCT T 609846-34-6, U 585-79-5  
RGT W 534-17-8 Cs2CO3  
PRO V 609846-35-7  
CAT 161265-03-8 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-diyl)bis[1,1-diphenyl-, 3375-31-3 Pd(OAc)2  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 95 deg C  
SUBSTAGE(3) 19 hours, 95 deg C

RX(30) RCT V 609846-35-7

STAGE(1)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

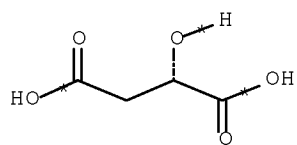
STAGE(2)  
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

PRO BV 609846-59-5

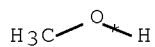
RX(504) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(7),  
RX(44)

RX(504) A + 2 B + E + O + U + CL ==>  
CM

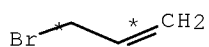
10/595943



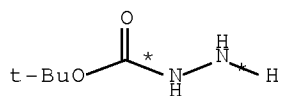
A



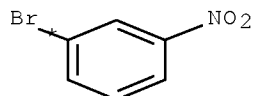
2 B



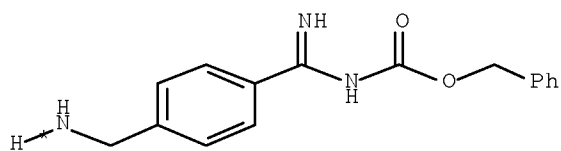
E



O



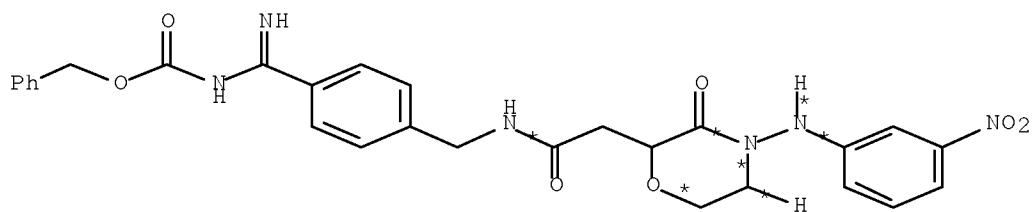
U



CL

2 HCl

8  
STEPS  
→



CM  
YIELD 87%

RX(1) RCT A 97-67-6, B 67-56-1  
RGT D 7719-09-7 SOCl2  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag2O

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PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K ~~7790-28-5~~ NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O ~~870-46-2~~  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(7) RCT T 609846-34-6, U 585-79-5  
RGT W 534-17-8 Cs2CO3  
PRO V 609846-35-7  
CAT 161265-03-8 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-diyl)bis[1,1-diphenyl-, 3375-31-3 Pd(OAc)2  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 95 deg C  
SUBSTAGE(3) 19 hours, 95 deg C

RX(44) RCT V 609846-35-7

STAGE(1)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)  
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature



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STAGE(3)

RCT CL 172348-75-3

RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2

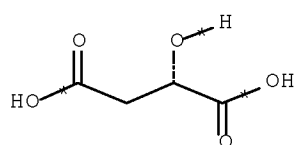
SOL 68-12-2 DMF

CON 100 minutes, room temperature

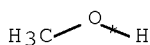
PRO CM 609846-74-4

RX(505) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(8),  
RX(46)

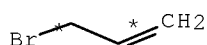
RX(505) 2 A + 4 B + 2 E + 2 O + 3 Z + CL ==>  
CP



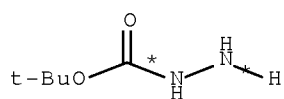
2 A



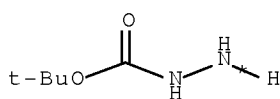
4 B



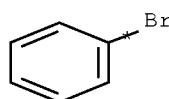
2 E



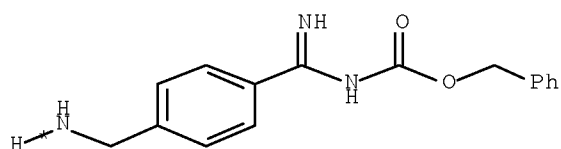
O



O



3 Z

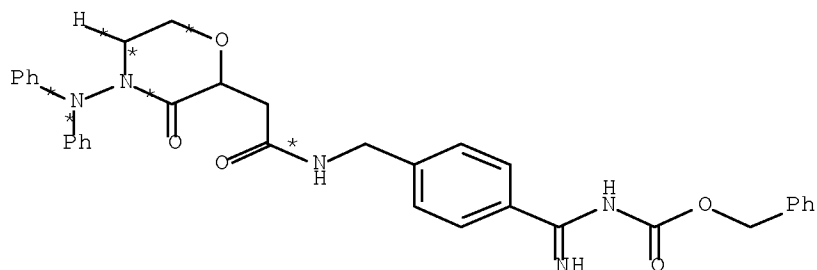


CL

● 2 HCl

8  
STEPS  
→

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CP

RX(1) RCT A 97-67-6, B 67-56-1  
 RGT D 7719-09-7 SOCl2  
 PRO C 617-55-0  
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
 RGT G 20667-12-3 Ag2O  
 PRO F 297749-53-2  
 SOL 108-88-3 PhMe  
 CON room temperature  
 NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
 RGT J 7529-22-8 Me-morpholineoxide  
 CAT 20816-12-0 OsO4  
 SOL 7732-18-5 Water, 109-99-9 THF  
 CON room temperature

STAGE(2)  
 RGT K 7790-28-5 NaIO4  
 SOL 7732-18-5 Water, 109-99-9 THF  
 CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
 PRO P 609846-32-4  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature -> 65 deg C  
 SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
 RGT R 1333-74-0 H2  
 PRO Q 609846-33-5  
 CAT 7440-05-3 Pd  
 SOL 109-99-9 THF  
 CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
 PRO T 609846-34-6  
 SOL 7732-18-5 Water  
 CON 7 hours, 60 deg C

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NTE key intermediate

RX(8) RCT T 609846-34-6, Z 108-86-1  
 RGT W 534-17-8 Cs2CO3  
 PRO AA 609846-36-8, AB 609847-53-2  
 CAT 161265-03-8 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-diyl)bis[1,1-diphenyl-, 3375-31-3 Pd(OAc)2  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) room temperature -> 95 deg C  
 SUBSTAGE(3) 19 hours, 95 deg C

RX(46) RCT AA 609846-36-8

STAGE(1)

RGT BW 1310-65-2 LiOH  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl  
 SOL 7732-18-5 Water  
 CON room temperature

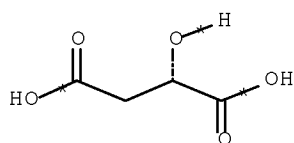
STAGE(3)

RCT CL 172348-75-3  
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium, 1-[bis(dimethylamino)methylene]-, 3-oxide, hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
 SOL 68-12-2 DMF  
 CON 100 minutes, room temperature

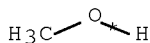
PRO CP 609846-76-6

RX(506) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(8), RX(71)

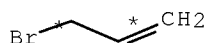
RX(506) 2 A + 4 B + 2 E + 2 O + 3 Z + CL + DM  
 ==> DQ



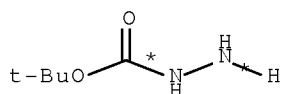
2 A



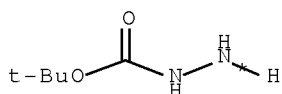
4 B



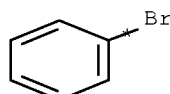
2 E



O

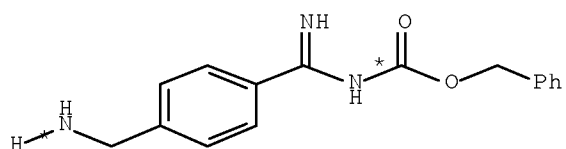


O



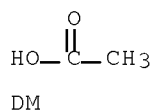
3 Z

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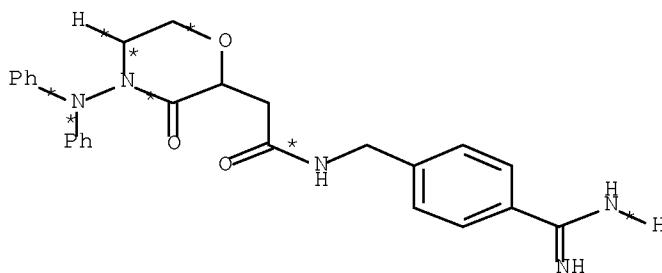
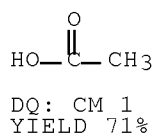


CL

● 2 HCl



8  
STEPS  
→



DQ: CM 2  
YIELD 71%

RX(1) RCT A 97-67-6, B 67-56-1  
RGT D 7719-09-7 SOCl2  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)

RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

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PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O ~~870-46-2~~  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(8) RCT T 609846-34-6, Z 108-86-1  
RGT W 534-17-8 Cs2CO3  
PRO AA 609846-36-8, AB 609847-53-2  
CAT 161265-03-8 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-diyl)bis[1,1-diphenyl-, 3375-31-3 Pd(OAc)2  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 95 deg C  
SUBSTAGE(3) 19 hours, 95 deg C

RX(71) RCT AA 609846-36-8

STAGE(1)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)  
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

STAGE(3)  
RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

STAGE(4)  
RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 7732-18-5 Water, 64-17-5 EtOH  
CON 45 minutes, room temperature

STAGE(5)  
RCT DM 64-19-7  
SOL 7732-18-5 Water, 67-56-1 MeOH

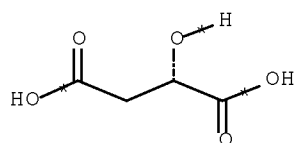
10/595943

CON room temperature

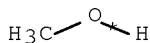
PRO DQ 609847-04-3

RX(507) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(8),  
RX(31)

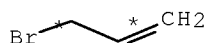
RX(507) 2 A + 4 B + 2 E + 2 O + 3 Z ==>  
BY



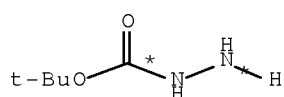
2 A



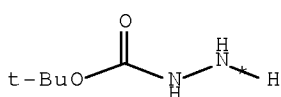
4 B



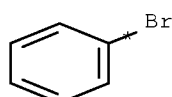
2 E



O

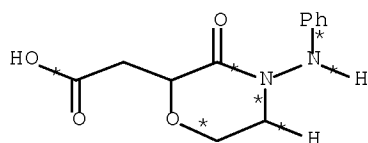


O



3 Z

8  
STEPS  
→



BY

RX(1) RCT A 97-67-6, B 67-56-1  
RGT D 7719-09-7 SOCl2  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)

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RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)

RGT K ~~7790-28-5~~ NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O ~~870-46-2~~  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(8) RCT T 609846-34-6, Z 108-86-1  
RGT W 534-17-8 Cs2CO3  
PRO AA 609846-36-8, AB 609847-53-2  
CAT 161265-03-8 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-diyl)bis[1,1-diphenyl-, 3375-31-3 Pd(OAc)2  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 95 deg C  
SUBSTAGE(3) 19 hours, 95 deg C

RX(31) RCT AB 609847-53-2

STAGE(1)

RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)

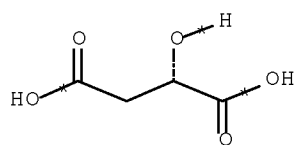
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

PRO BY ~~609846-61-9~~

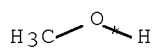
RX(508) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(8),  
RX(70)

RX(508) 2 A + 4 B + 2 E + 2 O + 3 Z + CL + DM  
==> DP

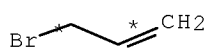
10/595943



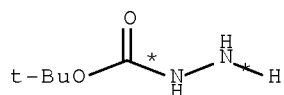
2 A



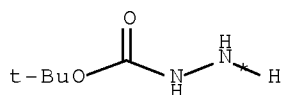
4 B



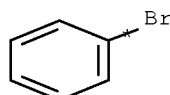
2 E



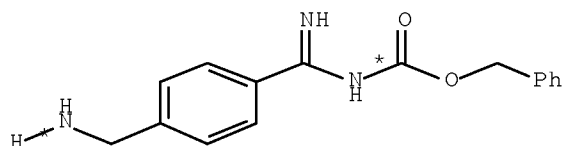
O



O

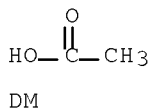


3 Z



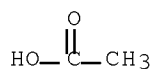
CL

● 2 HCl

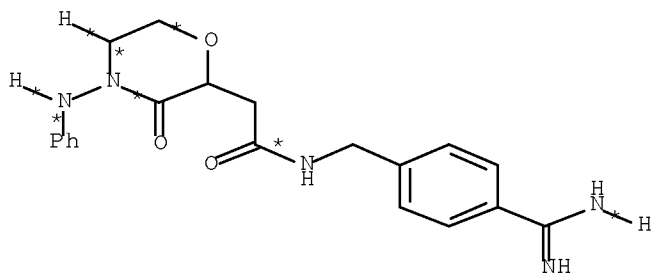


DM

8  
STEPS  
→



DP: CM 1  
YIELD 59%



DP: CM 2  
YIELD 59%

RX(1) RCT A 97-67-6, B 67-56-1  
RGT D 7719-09-7 SOCl<sub>2</sub>  
PRO C 617-55-0



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CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K ~~7790-28-5~~ NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O ~~870-46-2~~  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(8) RCT T 609846-34-6, Z 108-86-1  
RGT W 534-17-8 Cs2CO3  
PRO AA 609846-36-8, AB 609847-53-2  
CAT 161265-03-8 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-diyl)bis[1,1-diphenyl-, 3375-31-3 Pd(OAc)2  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 95 deg C  
SUBSTAGE(3) 19 hours, 95 deg C

RX(70) RCT AB 609847-53-2

STAGE(1)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

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STAGE(2)

RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

STAGE(3)

RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

STAGE(4)

RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 7732-18-5 Water, 64-17-5 EtOH  
CON 90 minutes, room temperature

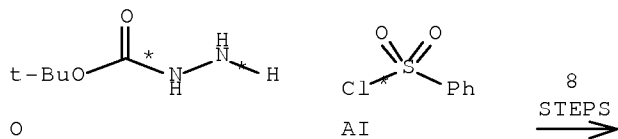
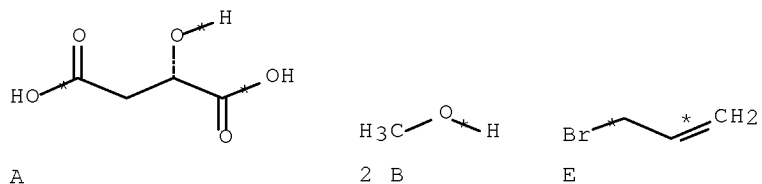
STAGE(5)

RCT DM 64-19-7  
SOL 7732-18-5 Water, 67-56-1 MeOH

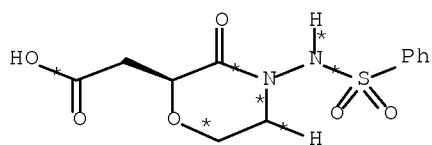
PRO DP 609847-02-1

RX(509) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(12),  
RX(35)

RX(509) A + 2 B + E + O + AI ==> CC



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CC

RX(1) RCT A 97-67-6, B 67-56-1  
RGT D 7719-09-7 SOCl<sub>2</sub>  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag<sub>2</sub>O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K 7790-28-5 NaIO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H<sub>2</sub>  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(12) RCT T 609846-34-6, AI 98-09-9  
PRO AK 609846-40-4

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SOL 110-86-1 Pyridine  
CON 20 hours, room temperature

RX(35) RCT AK 609846-40-4

STAGE(1)

RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

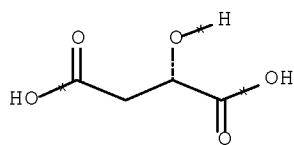
STAGE(2)

RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

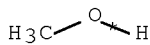
PRO CC 609846-65-3

RX(510) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(15),  
RX(53)

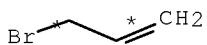
RX(510) A + 2 B + E + O + AN + CL ==>  
CW



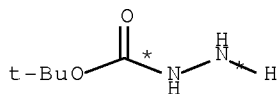
A



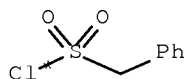
2 B



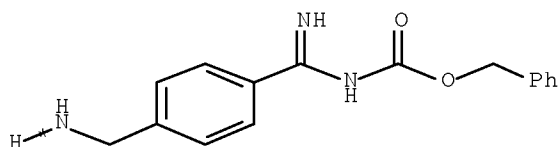
E



O



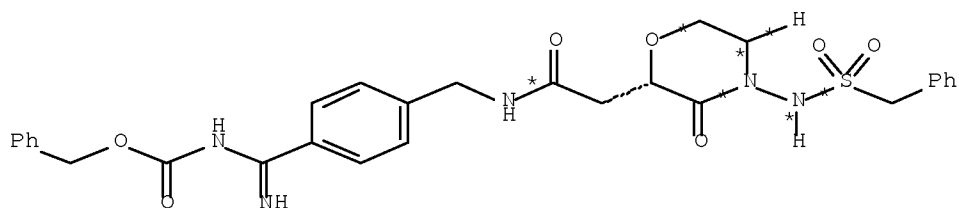
AN



CL

● 2 HCl

8  
STEPS  
→



RX(1) RCT A 97-67-6, B 67-56-1  
 RGT D 7719-09-7 SOCl<sub>2</sub>  
 PRO C 617-55-0  
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
 RGT G 20667-12-3 Ag<sub>2</sub>O  
 PRO F 297749-53-2  
 SOL 108-88-3 PhMe  
 CON room temperature  
 NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
 RGT J 7529-22-8 Me-morpholineoxide  
 CAT 20816-12-0 OsO<sub>4</sub>  
 SOL 7732-18-5 Water, 109-99-9 THF  
 CON room temperature

STAGE(2)  
 RGT K 7790-28-5 NaIO<sub>4</sub>  
 SOL 7732-18-5 Water, 109-99-9 THF  
 CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
 PRO P 609846-32-4  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature -> 65 deg C  
 SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
 RGT R 1333-74-0 H<sub>2</sub>  
 PRO Q 609846-33-5  
 CAT 7440-05-3 Pd  
 SOL 109-99-9 THF  
 CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
 PRO T 609846-34-6  
 SOL 7732-18-5 Water  
 CON 7 hours, 60 deg C

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NTE key intermediate

RX(15) RCT T 609846-34-6, AN 1939-99-7  
 PRO AP 609846-43-7  
 SOL 110-86-1 Pyridine  
 CON SUBSTAGE(1) 24 hours, room temperature  
 SUBSTAGE(2) room temperature -> 35 deg C  
 SUBSTAGE(3) 3 days, 35 deg C

RX(53) RCT AP 609846-43-7

STAGE(1)

RGT BW 1310-65-2 LiOH  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl  
 SOL 7732-18-5 Water  
 CON room temperature

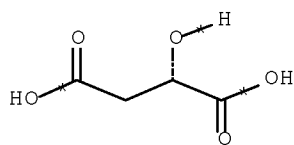
STAGE(3)

RCT CL 172348-75-3  
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
 1-[bis(dimethylamino)methylene]-, 3-oxide,  
 hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
 SOL 68-12-2 DMF  
 CON 100 minutes, room temperature

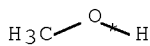
PRO CW 609846-83-5

RX(511) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(19),  
 RX(57)

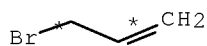
RX(511) A + 2 B + E + O + AU + CL ==>  
 DA



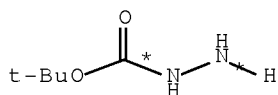
A



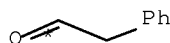
2 B



E

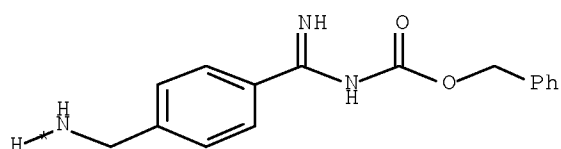


O



AU

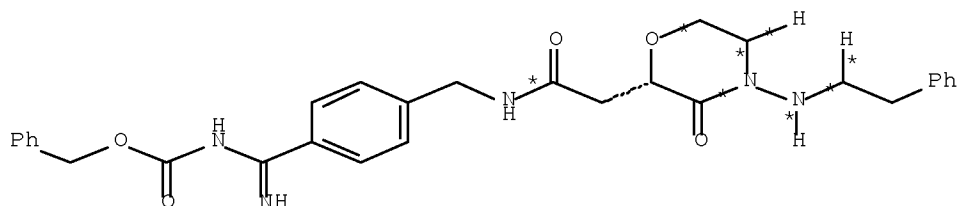
10/595943



CL

● 2 HCl

8  
STEPS  
→



DA

RX(1) RCT A ~~97-67-6~~, B 67-56-1  
RGT D 7719-09-7 SOCl2  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)

RGT K ~~7790-28-5~~ NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O ~~870-46-2~~  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C

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SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(19) RCT T 609846-34-6, AU 122-78-1

STAGE(1)

SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) overnight, 60 deg C

STAGE(2)

RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 2 hours, room temperature

PRO AW 609846-47-1

RX(57) RCT AW 609846-47-1

STAGE(1)

RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

STAGE(3)

RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

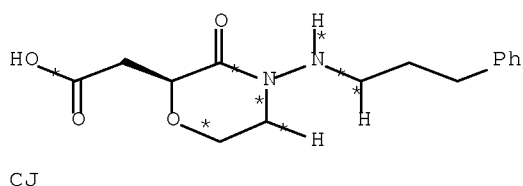
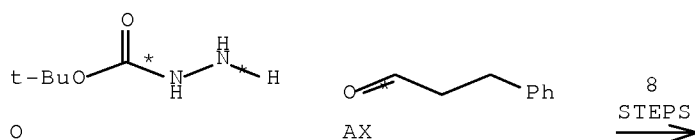
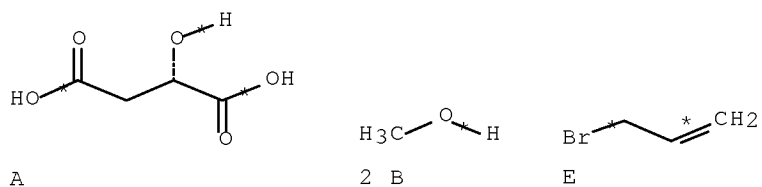
PRO DA 609846-87-9

RX(512) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(21),  
RX(42)

RX(512) A + 2 B + E + O + AX ==> CJ



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RX(1)      RCT    A 97-67-6, B 67-56-1  
               RGT    D 7719-09-7 SOCl2  
               PRO    C 617-55-0  
               CON    room temperature  
  
 RX(2)      RCT    C 617-55-0, E 106-95-6  
               RGT    G 20667-12-3 Ag2O  
               PRO    F 297749-53-2  
               SOL    108-88-3 PhMe  
               CON    room temperature  
               NTE    other product also detected

RX(3)      RCT    F 297749-53-2

STAGE(1)

RGT    J 7529-22-8 Me-morpholineoxide  
 CAT    20816-12-0 OsO4  
 SOL    7732-18-5 Water, 109-99-9 THF  
 CON    room temperature

STAGE(2)

RGT    K 7790-28-5 NaIO4  
 SOL    7732-18-5 Water, 109-99-9 THF  
 CON    room temperature

PRO    I 441764-54-1

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RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

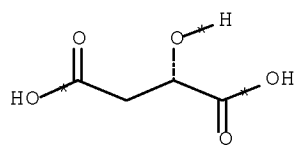
RX(21) RCT T 609846-34-6, AX 104-53-0  
  
STAGE(1)  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) 5 hours, 70 deg C  
  
STAGE(2)  
RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 3 hours, room temperature

PRO BA 609846-50-6

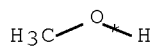
RX(42) RCT BA 609846-50-6  
  
STAGE(1)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature  
  
STAGE(2)  
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature  
  
PRO CJ 609846-72-2

RX(513) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(23),  
RX(62)  
RX(513) A + 2 B + E + O + BB + CL ==>  
DF

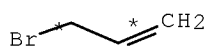
10/595943



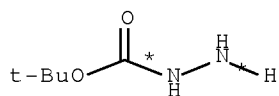
A



2 B



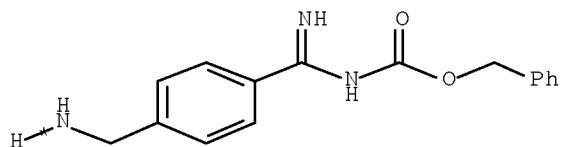
E



O



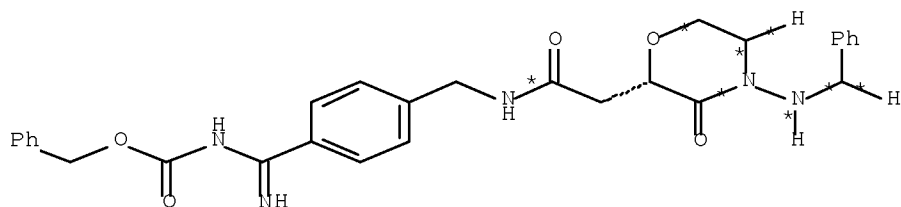
BB



CL

● 2 HCl

8  
STEPS  
→



DF

RX(1) RCT A 97-67-6, B 67-56-1  
RGT D 7719-09-7 SOCl2  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe

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CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)

RGT K ~~7790-28-5~~ NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O ~~870-46-2~~  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(23) RCT T 609846-34-6, BB 100-52-7

STAGE(1)

RGT BD 1125-88-8 PhCH(OMe)2  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 80 deg C  
SUBSTAGE(2) 2 days, 80 deg C

STAGE(2)

RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 5 minutes, room temperature

PRO BE 609846-52-8

RX(62) RCT BE 609846-52-8

STAGE(1)

RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

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STAGE(2)

RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

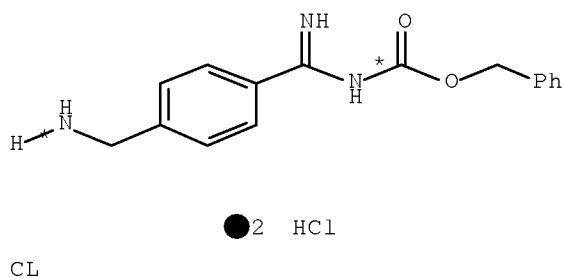
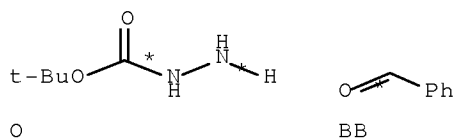
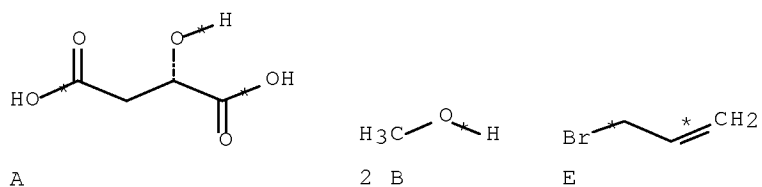
STAGE(3)

RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

PRO DF 609846-92-6

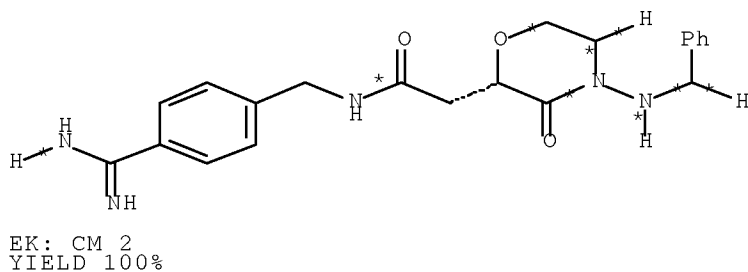
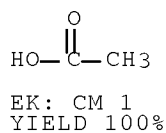
RX(514) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(23),  
RX(87)

RX(514) A + 2 B + E + O + BB + CL + DM ==>  
EK



8  
STEPS  
➔

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RX(1) RCT A 97-67-6, B 67-56-1  
RGT D 7719-09-7 SOCl2  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

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RX(23) RCT T 609846-34-6, BB 100-52-7

STAGE(1)

RGT BD 1125-88-8 PhCH(OMe)2  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 80 deg C  
SUBSTAGE(2) 2 days, 80 deg C

STAGE(2)

RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 5 minutes, room temperature

PRO BE 609846-52-8

RX(87) RCT BE 609846-52-8

STAGE(1)

RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

STAGE(3)

RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

STAGE(4)

RGT EG 1493-13-6 F3CSO2H, EH 100-66-3 PhOMe  
SOL 75-09-2 CH2Cl2  
CON 15 minutes, 0 deg C

STAGE(5)

RGT EI 121-44-8 Et3N  
CON neutralized

STAGE(6)

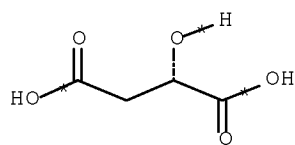
RCT DM 64-19-7  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

PRO EK 609847-35-0

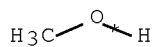
RX(515) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(24),  
RX(63)

RX(515) A + 2 B + E + O + 2 BF + CL ==>  
DG

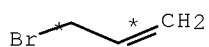
10/595943



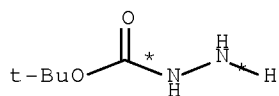
A



2 B



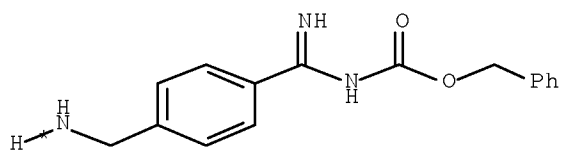
E



O



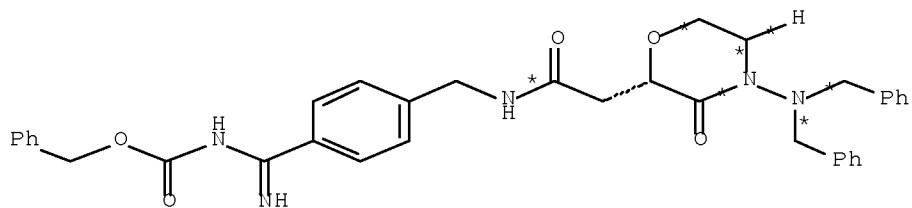
2 BF



CL

2 HCl

8  
STEPS  
→



DG

RX(1) RCT A 97-67-6, B 67-56-1  
RGT D 7719-09-7 SOCl2  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2



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SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K ~~7790-28-5~~ NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O ~~870-46-2~~  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(24) RCT T 609846-34-6, BF 100-39-0  
RGT BH 7087-68-5 EtN(Pr-i)2, BI 144-55-8 NaHCO3  
PRO BG 609846-53-9  
CAT ~~10377-51-2~~ LiI  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) room temperature -> 50 deg C  
SUBSTAGE(2) 7 hours, 50 deg C

RX(63) RCT BG 609846-53-9

STAGE(1)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)  
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

STAGE(3)  
RCT CL 172348-75-3

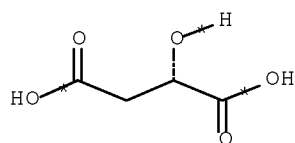
10/595943

RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)<sub>2</sub>  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

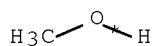
PRO DG 609846-93-7

RX(516) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(25),  
RX(64)

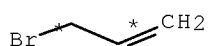
RX(516) A + 2 B + E + O + BL + CL ==>  
DH



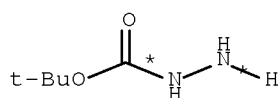
A



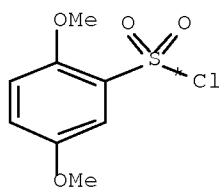
2 B



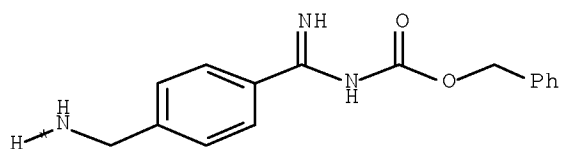
E



O



BL

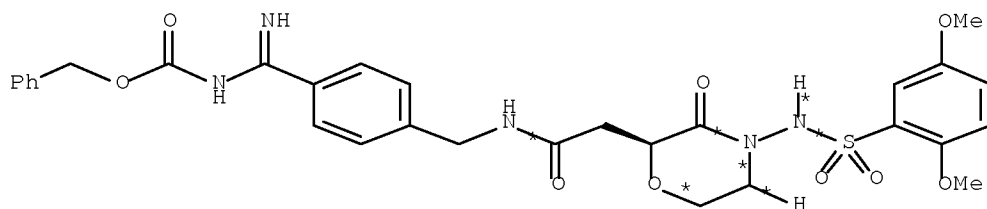


CL

● 2 HCl

8  
STEPS  
→

10/595943



DH

RX(1) RCT A ~~97-67-6~~, B 67-56-1  
RGT D 7719-09-7 SOCl<sub>2</sub>  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag<sub>2</sub>O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K ~~7790-28-5~~ NaIO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O ~~870-46-2~~  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H<sub>2</sub>  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

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RX(25) RCT T 609846-34-6, BL 1483-28-9  
 PRO BM 609846-54-0  
 SOL 110-86-1 Pyridine  
 CON 24 hours, room temperature

RX(64) RCT BM 609846-54-0

STAGE(1)

RGT BW 1310-65-2 LiOH  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl  
 SOL 7732-18-5 Water  
 CON room temperature

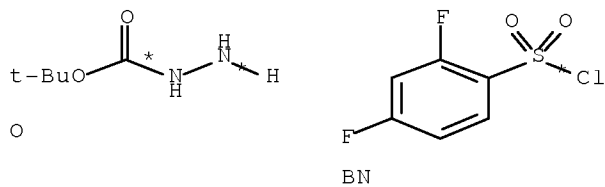
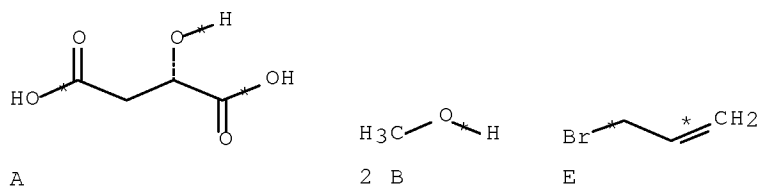
STAGE(3)

RCT CL 172348-75-3  
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
 1-[bis(dimethylamino)methylene]-, 3-oxide,  
 hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
 SOL 68-12-2 DMF  
 CON 100 minutes, room temperature

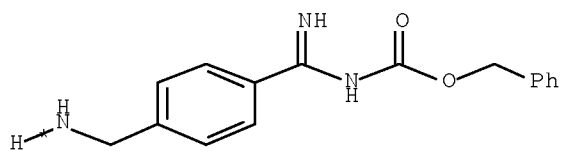
PRO DH 609846-94-8

RX(517) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(26),  
 RX(65)

RX(517) A + 2 B + E + O + BN + CL ==>  
 DI



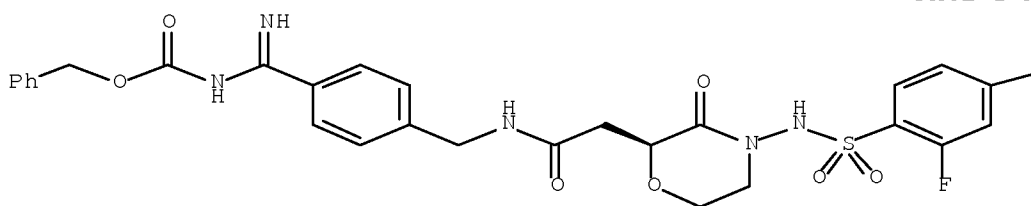
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CL

● 2 HCl

8  
STEPS  
→



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— F  
DI

RX(1)	RCT	A 97-57-6, B 67-56-1
	RGT	D 7719-09-7 SOC12
	PRO	C 617-55-0
	CON	room temperature
RX(2)	RCT	C 617-55-0, E 106-95-6
	RGT	G 20667-12-3 Ag2O
	PRO	F 297749-53-2
	SOL	108-88-3 PhMe
	CON	room temperature
	NTE	other product also detected
RX(3)	RCT	F 297749-53-2

```
STAGE(1)
  RGT    J 7529-22-8 Me-morpholineoxide
  CAT    20816-12-0 OsO4
  SOL    7732-18-5 Water, 109-99-9 THF
  CON    room temperature
```

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STAGE(2)

RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(26) RCT T 609846-34-6, BN 13918-92-8  
PRO BO 609846-55-1  
SOL 110-86-1 Pyridine  
CON 24 hours, room temperature

RX(65) RCT BO 609846-55-1

STAGE(1)

RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

STAGE(3)

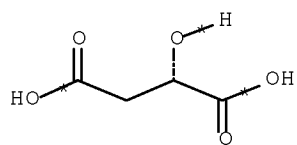
RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

PRO DI 609846-95-9

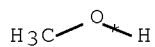
RX(518) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(27),  
RX(66)

RX(518) A + 2 B + E + O + BP + CL ==>  
DJ

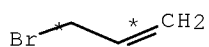
10/595943



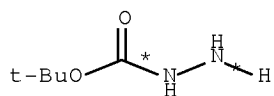
A



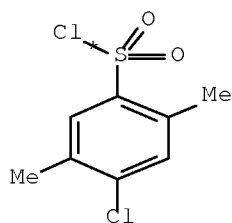
2 B



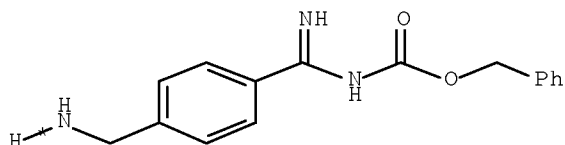
E



O



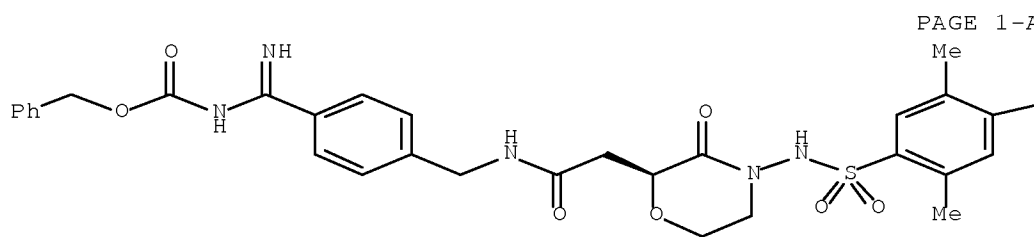
BP



CL

● 2 HCl

8  
STEPS  
→



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DJ

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RX(1) RCT A ~~97-67-6~~, B 67-56-1  
RGT D 7719-09-7 SOCl<sub>2</sub>  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag<sub>2</sub>O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K ~~7790-28-5~~ NaIO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O ~~870-46-2~~  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H<sub>2</sub>  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(27) RCT T 609846-34-6, BP 88-49-3  
PRO BQ 609846-56-2  
SOL 110-86-1 Pyridine  
CON 24 hours, room temperature

RX(66) RCT BQ 609846-56-2

STAGE(1)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)



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RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

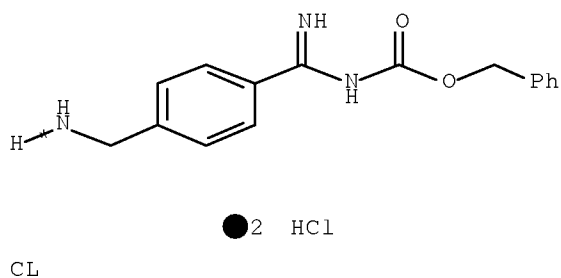
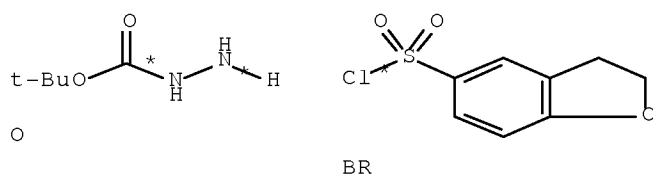
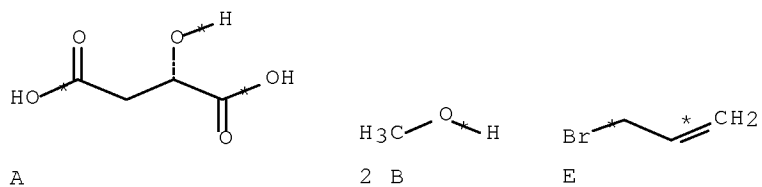
STAGE(3)

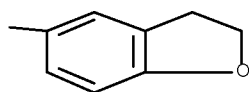
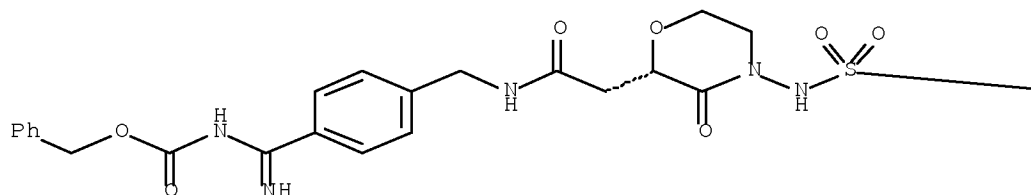
RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

PRO DJ 609846-96-0

RX(519) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(28),  
RX(67)

RX(519) A + 2 B + E + O + BR + CL ==>  
DK





DK

RX(1)      RCT    A 97-67-6, B 67-56-1  
              RGT    D 7719-09-7 SOCl2  
              PRO    C 617-55-0  
              CON    room temperature

RX(2)      RCT    C 617-55-0, E 106-95-6  
              RGT    G 20667-12-3 Ag2O  
              PRO    F 297749-53-2  
              SOL    108-88-3 PhMe  
              CON    room temperature  
              NTE    other product also detected

RX(3)      RCT    F 297749-53-2

             STAGE(1)  
                  RGT    J 7529-22-8 Me-morpholineoxide  
                  CAT    20816-12-0 OsO4  
                  SOL    7732-18-5 Water, 109-99-9 THF  
                  CON    room temperature

             STAGE(2)  
                  RGT    K 7790-28-5 NaIO4  
                  SOL    7732-18-5 Water, 109-99-9 THF  
                  CON    room temperature

             PRO    I 441764-54-1

RX(4)      RCT    I 441764-54-1, O 870-46-2  
              PRO    P 609846-32-4  
              SOL    108-88-3 PhMe  
              CON    SUBSTAGE(1) room temperature -> 65 deg C  
                      SUBSTAGE(2) overnight, 65 deg C

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RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(28) RCT T 609846-34-6, BR 115010-11-2  
PRO BS 609846-57-3  
SOL 110-86-1 Pyridine  
CON 90 minutes, room temperature

RX(67) RCT BS 609846-57-3

STAGE(1)

RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

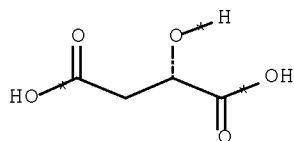
STAGE(3)

RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

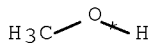
PRO DK 609846-97-1

RX(520) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(29),  
RX(68)

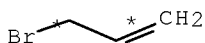
RX(520) A + 2 B + E + O + BT + CL ==>  
DL



A

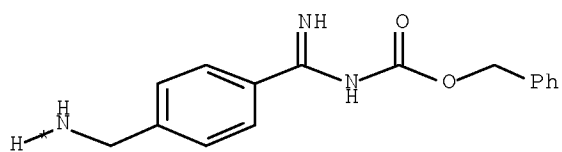
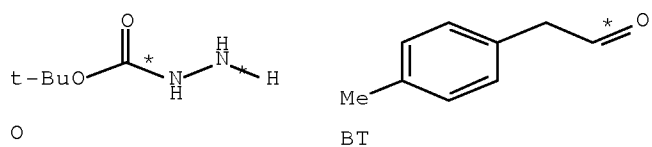


2 B



E

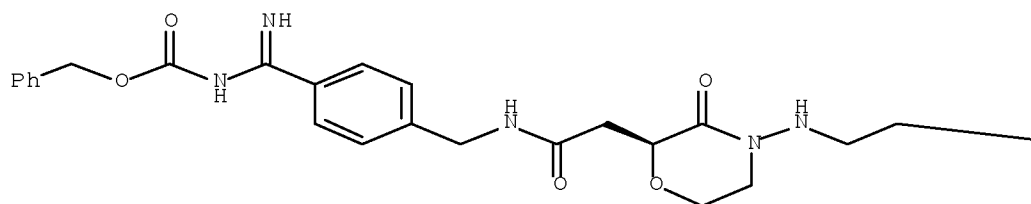
10/595943



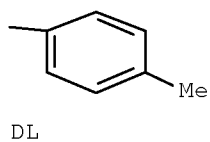
● 2 HCl

8  
STEPS  
→

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RX(1) RCT A 97-67-6, B 67-56-1  
 RGT D 7719-09-7 SOCl<sub>2</sub>  
 PRO C 617-55-0  
 CON room temperature

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RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(29) RCT T 609846-34-6, BT 104-09-6

STAGE(1)  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) overnight, 75 deg C

STAGE(2)  
RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 24 hours, room temperature

PRO BU 609846-58-4

RX(68) RCT BU 609846-58-4

STAGE(1)  
RGT BW 1310-65-2 LiOH

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SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

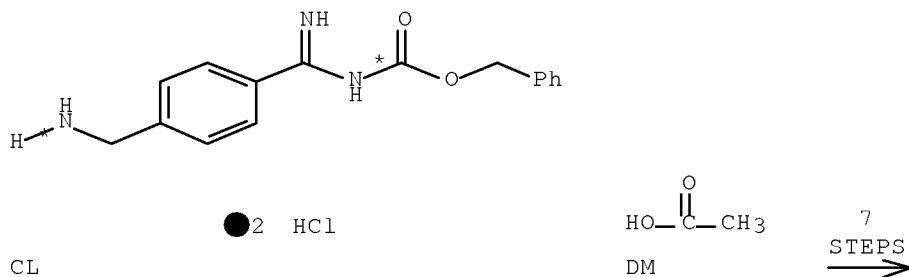
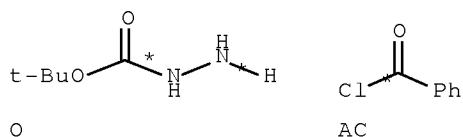
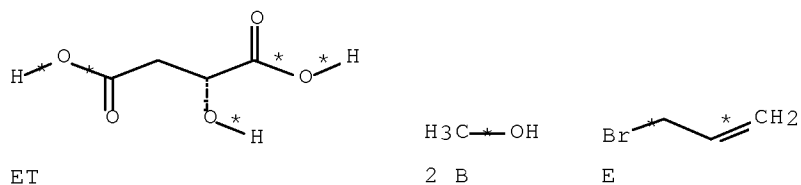
STAGE(3)

RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

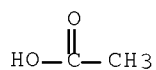
PRO DL 609846-98-2

RX(572) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(9), RX(47),  
RX(72)

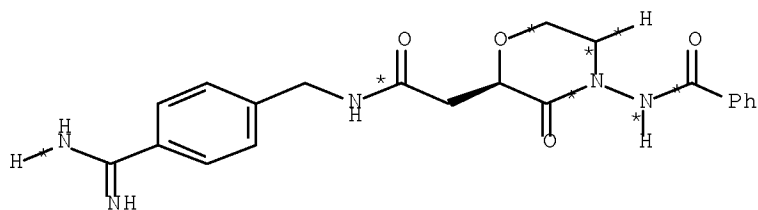
RX(572) ET + 2 B + E + O + AC + CL + DM ==>  
DR



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DR: CM 1  
YIELD 84%



DR: CM 2  
YIELD 84%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2

CON room temperature

STAGE(2)

RCT E 106-95-6

RGT G 20667-12-3 Ag2O

SOL 108-88-3 PhMe

CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide

CAT 20816-12-0 OsO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

PRO ES 609847-51-0

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C

SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0

RGT R 1333-74-0 H2

PRO AG 609847-50-9

CAT 7440-05-3 Pd

SOL 109-99-9 THF

CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9

PRO AD 609847-52-1

SOL 7732-18-5 Water

CON 7 hours, 60 deg C

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NTE key intermediate

RX(9) RCT AC 98-88-4, AD 609847-52-1

STAGE(1)

SOL 110-86-1 Pyridine

CON 25 minutes, room temperature

STAGE(2)

SOL 7732-18-5 Water

PRO AE 609846-37-9

RX(47) RCT AE 609846-37-9

STAGE(1)

RGT BW 1310-65-2 LiOH

SOL 7732-18-5 Water, 67-56-1 MeOH

CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl

SOL 7732-18-5 Water

CON room temperature

STAGE(3)

RCT CL 172348-75-3

RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2

SOL 68-12-2 DMF

CON 100 minutes, room temperature

PRO CQ 609846-77-7

RX(72) RCT CQ 609846-77-7

STAGE(1)

RGT R 1333-74-0 H2

CAT 7440-05-3 Pd

SOL 7732-18-5 Water, 64-17-5 EtOH

CON 65 minutes, room temperature

STAGE(2)

RCT DM 64-19-7

SOL 7732-18-5 Water, 67-56-1 MeOH

CON room temperature

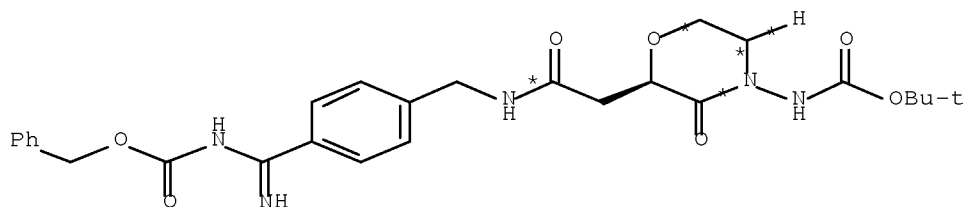
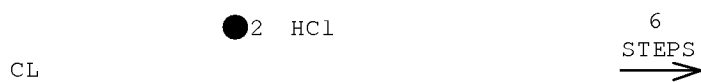
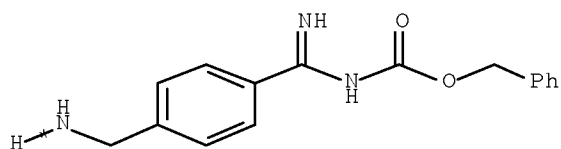
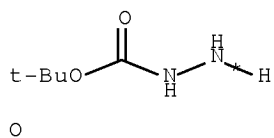
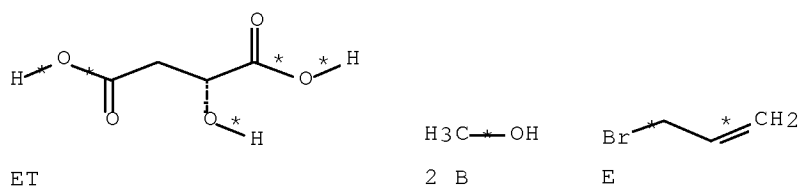
PRO DR 609847-06-5

RX(573) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(10), RX(33), RX(48)

RX(573) ET + 2 B + E + O + CL ==> CR



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CR

RX(95)                      RCT                      ET 636-61-3, B 67-56-1

STAGE(1)

RGT                      D 7719-09-7 SOCl2  
CON                      room temperature

STAGE(2)

RCT                      E 106-95-6  
RGT                      G 20667-12-3 Ag2O

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SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H2  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(10) RCT AG 609847-50-9  
PRO AH 609846-38-0  
SOL 108-88-3 PhMe  
CON 3 days, reflux

RX(33) RCT AH 609846-38-0

STAGE(1)

RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

PRO CA 609846-63-1

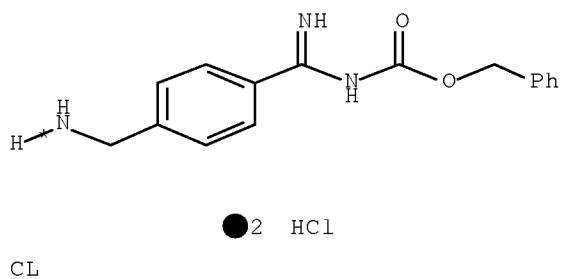
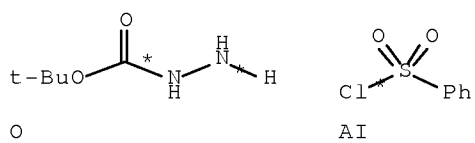
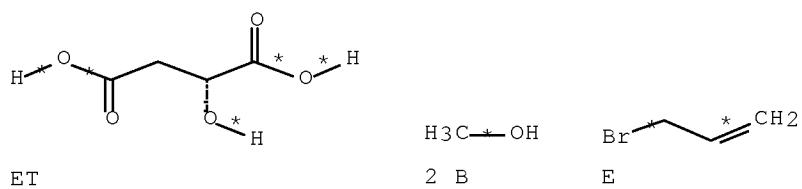
RX(48) RCT CA 609846-63-1, CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
PRO CR 609846-78-8  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

RX(574) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(11), RX(34),  
RX(49)

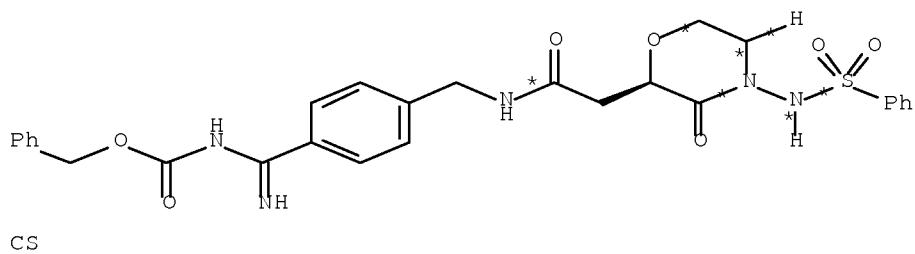
RX(574) ET + 2 B + E + O + AI + CL ==>

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CS



7  
STEPS  
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RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2  
CON room temperature

## STAGE(2)

RCT E 106-95-6  
RGT G 20667-12-3 Ag2O  
SOL 108-88-3 PhMe  
CON room temperature

## STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

## STAGE(4)

RGT K ~~7790-28-5~~ NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O ~~870-46-2~~, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H2  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(11) RCT AI 98-09-9, AD 609847-52-1  
PRO AJ 609846-39-1  
SOL 110-86-1 Pyridine  
CON 20 hours, room temperature

RX(34) RCT AJ 609846-39-1

## STAGE(1)

RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

## STAGE(2)

RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

PRO CB 609846-64-2

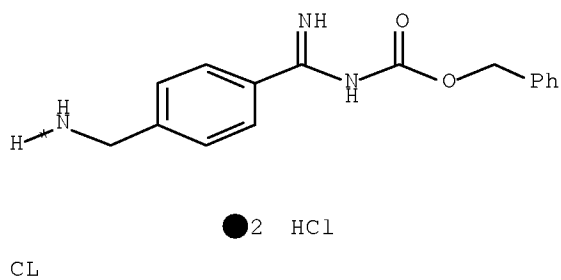
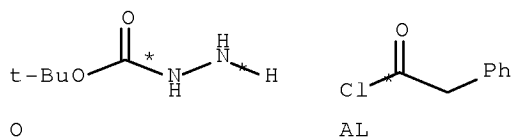
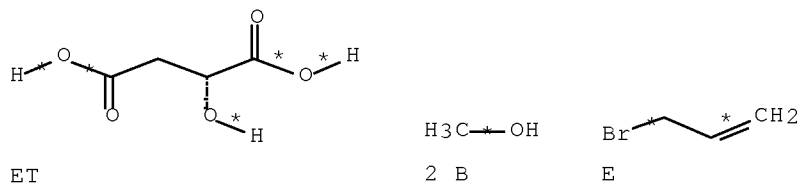
RX(49) RCT CB 609846-64-2, CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,

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1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
PRO CS 609846-79-9  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

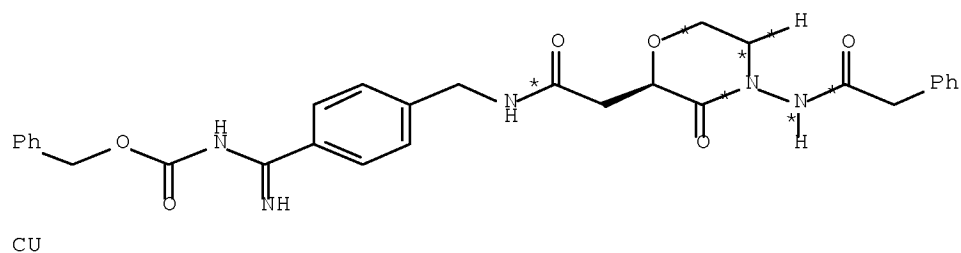
RX(575) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(13), RX(36),  
RX(51)

RX(575) ET + 2 B + E + O + AL + CL ==>  
CU



7  
STEPS  
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RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl<sub>2</sub>  
CON room temperature

STAGE(2)

RCT E 106-95-6  
RGT G 20667-12-3 Ag<sub>2</sub>O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H<sub>2</sub>  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(13) RCT AL 103-80-0, AD 609847-52-1  
PRO AM 609846-41-5

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SOL 110-86-1 Pyridine  
CON 29 hours, room temperature

RX(36) RCT AM 609846-41-5

STAGE(1)

RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)

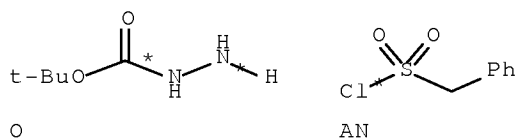
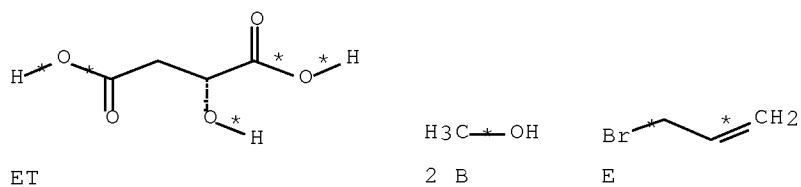
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

PRO CD 609846-66-4

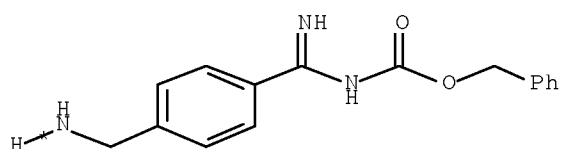
RX(51) RCT CD 609846-66-4, CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
PRO CU 609846-81-3  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

RX(576) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(14), RX(37),  
RX(52)

RX(576) ET + 2 B + E + O + AN + CL ==>  
CV



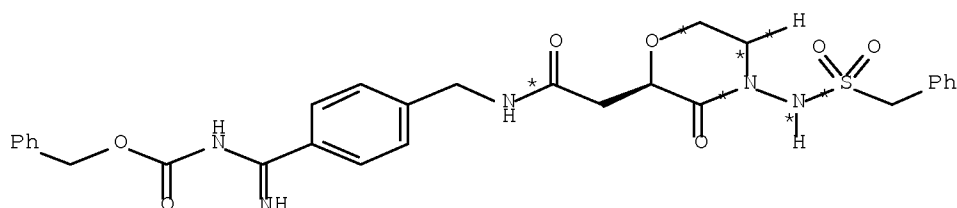
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CL

● 2 HCl

7  
STEPS  
→



CV

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2  
CON room temperature

STAGE(2)

RCT E 106-95-6  
RGT G 20667-12-3 Ag2O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C



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RX(94) RCT ES 609847-51-0  
 RGT R 1333-74-0 H2  
 PRO AG 609847-50-9  
 CAT 7440-05-3 Pd  
 SOL 109-99-9 THF  
 CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
 PRO AD 609847-52-1  
 SOL 7732-18-5 Water  
 CON 7 hours, 60 deg C  
 NTE key intermediate

RX(14) RCT AN 1939-99-7, AD 609847-52-1  
 PRO AO 609846-42-6  
 SOL 110-86-1 Pyridine  
 CON 24 hours, room temperature

RX(37) RCT AO 609846-42-6

STAGE(1)

RGT BW 1310-65-2 LiOH  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON room temperature

STAGE(2)

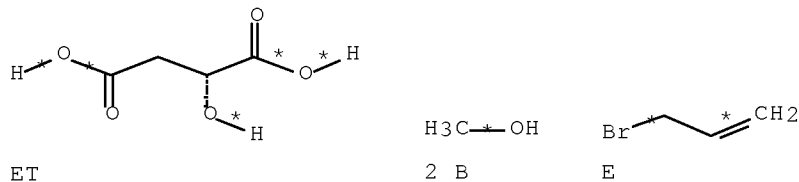
RGT BX 7647-01-0 HCl  
 SOL 7732-18-5 Water  
 CON room temperature

PRO CE 609846-67-5

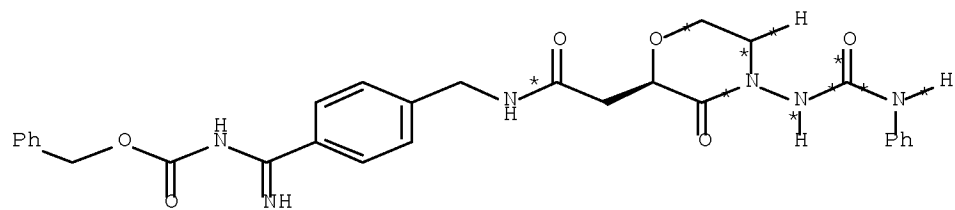
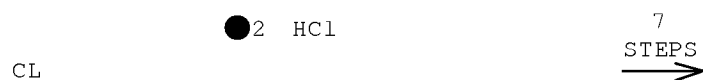
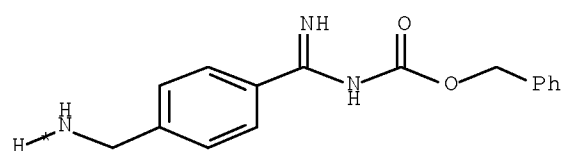
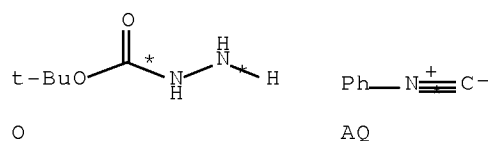
RX(52) RCT CE 609846-67-5, CL 172348-75-3  
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
 1-[bis(dimethylamino)methylene]-, 3-oxide,  
 hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
 PRO CV 609846-82-4  
 SOL 68-12-2 DMF  
 CON 100 minutes, room temperature

RX(577) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(16), RX(38),  
 RX(54)

RX(577) ET + 2 B + E + O + AQ + CL ==>  
 CX



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CX

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl<sub>2</sub>  
CON room temperature

STAGE(2)

RCT E 106-95-6  
RGT G 20667-12-3 Ag<sub>2</sub>O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)

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RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O ~~870-46-2~~, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H2  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(16) RCT AQ 931-54-4, AD 609847-52-1  
  
STAGE(1)  
SOL 108-88-3 PhMe  
CON 25 hours, room temperature  
  
STAGE(2)  
RGT B 67-56-1 MeOH  
SOL 67-56-1 MeOH  
CON 5 minutes, 40 deg C

PRO AR 609846-44-8

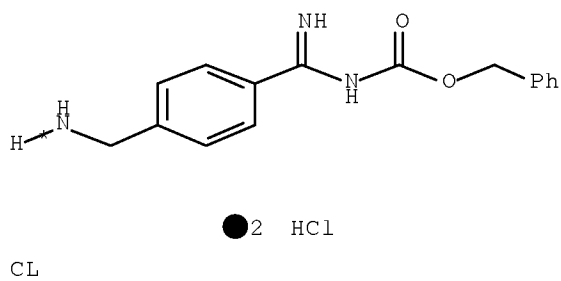
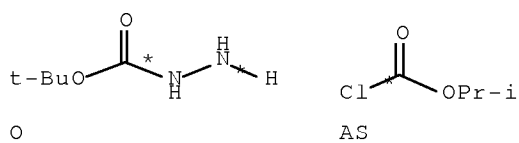
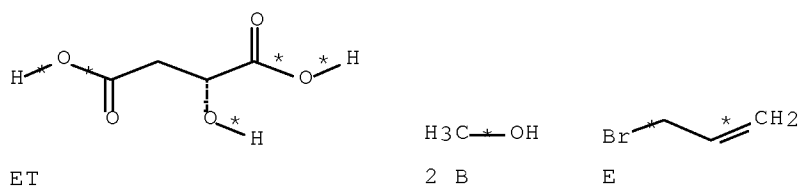
RX(38) RCT AR 609846-44-8  
  
STAGE(1)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature  
  
STAGE(2)  
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

PRO CF 609846-68-6

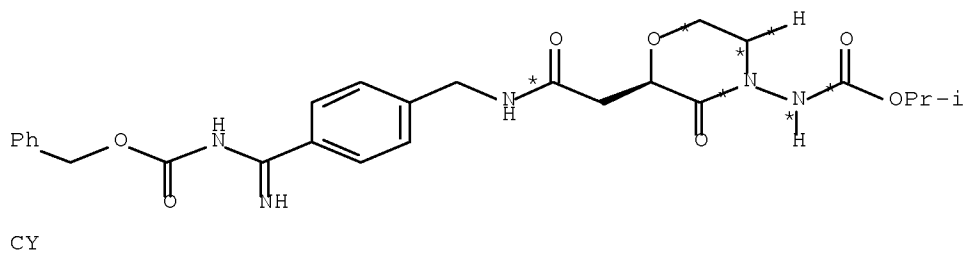
RX(54) RCT CF 609846-68-6, CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
PRO CX ~~609846-84-6~~  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

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RX(578) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(17), RX(39),  
 RX(55)  
 RX(578) ET + 2 B + E + O + AS + CL ==>  
 CY



7  
 STEPS  
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RX(95) RCT ET 636-61-3, B 67-56-1

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STAGE(1)

RGT D 7719-09-7 SOCl<sub>2</sub>  
CON room temperature

STAGE(2)

RCT E 106-95-6  
RGT G 20667-12-3 Ag<sub>2</sub>O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)

RGT K ~~7790-28-5~~ NaIO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O ~~870-46-2~~, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H<sub>2</sub>  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(17) RCT AS 108-23-6, AD 609847-52-1  
PRO AT 609846-45-9  
SOL 108-88-3 PhMe, 110-86-1 Pyridine  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 4 hours

RX(39) RCT AT 609846-45-9

STAGE(1)

RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

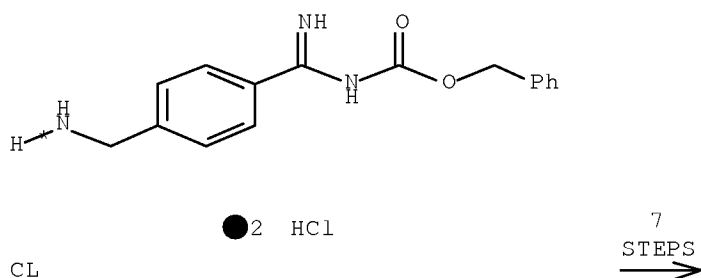
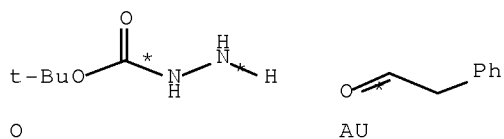
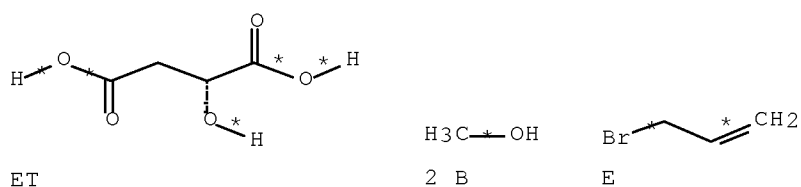
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PRO CG 609846-69-7

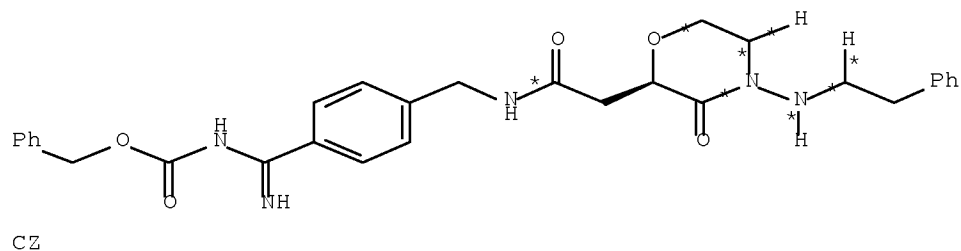
RX(55) RCT CG 609846-69-7, CL 172348-75-3  
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
 1-[bis(dimethylamino)methylene]-, 3-oxide,  
 hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
 PRO CY 609846-85-7  
 SOL 68-12-2 DMF  
 CON 100 minutes, room temperature

RX(579) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(18), RX(40),  
 RX(56)

RX(579) ET + 2 B + E + O + AU + CL ==>  
 CZ



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RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl<sub>2</sub>  
CON room temperature

STAGE(2)

RCT E 106-95-6  
RGT G 20667-12-3 Ag<sub>2</sub>O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H<sub>2</sub>  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(18) RCT AU 122-78-1, AD 609847-52-1

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STAGE(1)  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) overnight, 60 deg C

STAGE(2)  
 RGT R 1333-74-0 H2  
 CAT 7440-05-3 Pd  
 SOL 109-99-9 THF  
 CON 2 hours, room temperature

PRO AV 609846-46-0

RX(40) RCT AV 609846-46-0

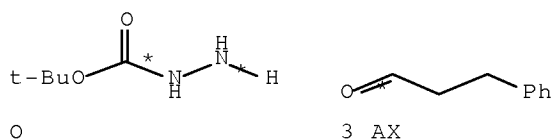
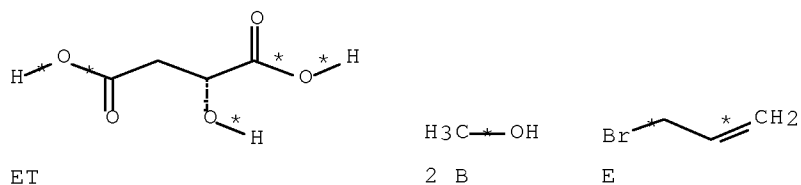
STAGE(1)  
 RGT BW 1310-65-2 LiOH  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON room temperature

STAGE(2)  
 RGT BX 7647-01-0 HCl  
 SOL 7732-18-5 Water  
 CON room temperature

PRO CH 609846-70-0

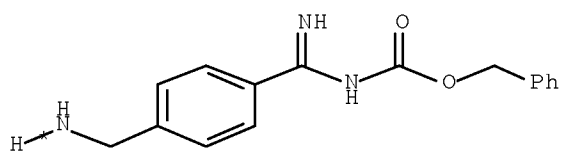
RX(56) RCT CH 609846-70-0, CL 172348-75-3  
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
 1-[bis(dimethylamino)methylene]-, 3-oxide,  
 hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
 PRO CZ 609846-86-8  
 SOL 68-12-2 DMF  
 CON 100 minutes, room temperature

RX(580) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(20), RX(41),  
 RX(58)  
 RX(580) ET + 2 B + E + O + 3 AX + CL ==>  
 DB





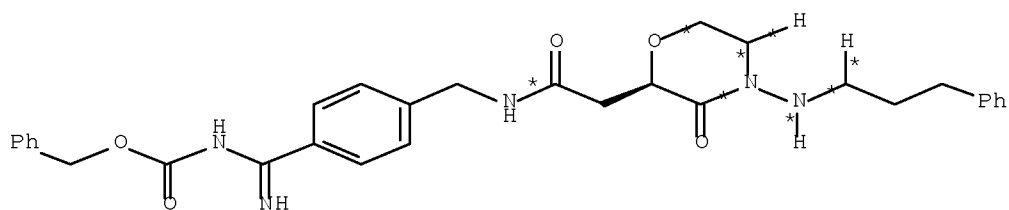
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CL

● 2 HCl

7  
STEPS  
➔



DB

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2

CON room temperature

STAGE(2)

RCT E 106-95-6

RGT G 20667-12-3 Ag2O

SOL 108-88-3 PhMe

CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide

CAT 20816-12-0 OsO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

PRO ES 609847-51-0

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```
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
    SUBSTAGE(2) overnight, 65 deg C

RX(94)  RCT  ES 609847-51-0
        RGT  R 1333-74-0 H2
        PRO  AG 609847-50-9
        CAT  7440-05-3 Pd
        SOL  109-99-9 THF
        CON  18 hours, room temperature

RX(97)  RCT  AG 609847-50-9
        PRO  AD 609847-52-1
        SOL  7732-18-5 Water
        CON  7 hours, 60 deg C
        NTE  key intermediate

RX(20)  RCT  AX 104-53-0, AD 609847-52-1

        STAGE(1)
            SOL 108-88-3 PhMe
            CON SUBSTAGE(1) room temperature
                SUBSTAGE(2) 24 hours, 70 deg C

        STAGE(2)
            RGT R 1333-74-0 H2
            CAT 7440-05-3 Pd
            SOL 109-99-9 THF
            CON 70 minutes, room temperature

        PRO  AY 609846-48-2, AZ 609846-49-3

RX(41)  RCT  AY 609846-48-2

        STAGE(1)
            RGT BW 1310-65-2 LiOH
            SOL 7732-18-5 Water, 67-56-1 MeOH
            CON room temperature

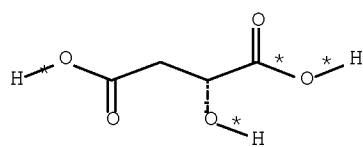
        STAGE(2)
            RGT BX 7647-01-0 HCl
            SOL 7732-18-5 Water
            CON room temperature

        PRO  CI 609846-71-1

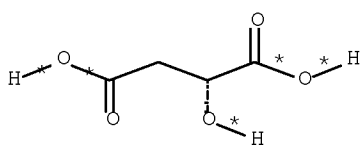
RX(58)  RCT  CI 609846-71-1, CL 172348-75-3
        RGT  CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
            1-[bis(dimethylamino)methylene]-, 3-oxide,
            hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
        PRO  DB 609846-88-0
        SOL  68-12-2 DMF
        CON  100 minutes, room temperature

RX(581) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(20), RX(60),
        RX(85)
RX(581)  2 ET + 2 B + 2 E + 2 O + 3 AX + CL +
        DM ==> EE
```

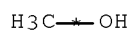
10/595943



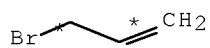
ET



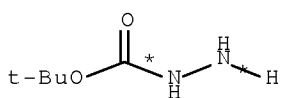
ET



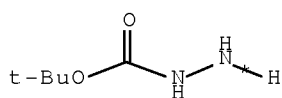
2 B



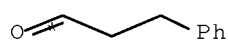
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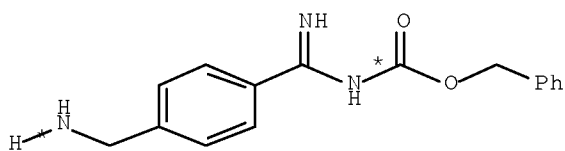
O



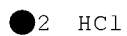
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3 AX

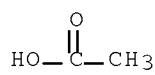


CL



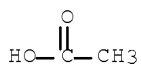
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HCl



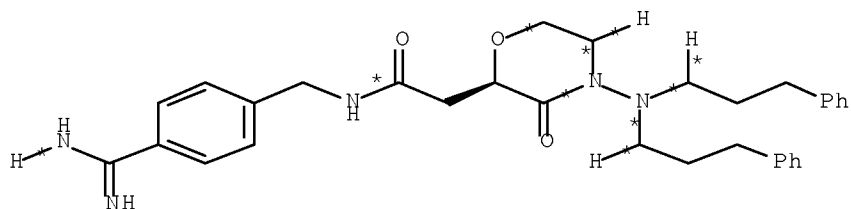
DM

7  
STEPS  
→



EE: CM 1  
YIELD 75%

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EE: CM 2  
YIELD 75%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2  
CON room temperature

STAGE(2)

RCT E 106-95-6  
RGT G 20667-12-3 Ag2O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H2  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(20) RCT AX 104-53-0, AD 609847-52-1

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STAGE(1)  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) 24 hours, 70 deg C

STAGE(2)  
RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 70 minutes, room temperature

PRO AY 609846-48-2, AZ 609846-49-3

RX(60) RCT AZ 609846-49-3

STAGE(1)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)  
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

STAGE(3)  
RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

PRO DD 609846-90-4

RX(85) RCT DD 609846-90-4

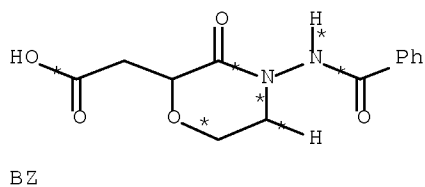
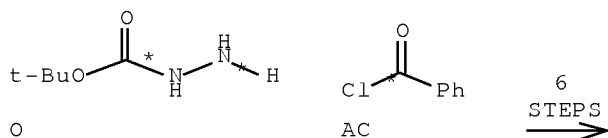
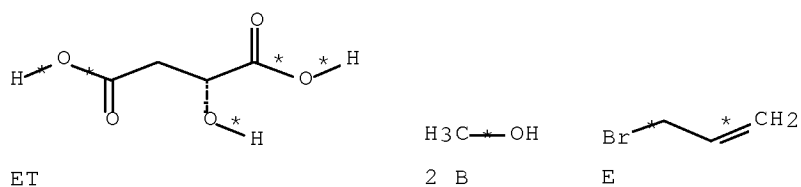
STAGE(1)  
RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 7732-18-5 Water, 64-17-5 EtOH, 109-99-9 THF  
CON 3 hours, room temperature

STAGE(2)  
RCT DM 64-19-7  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

PRO EE 609847-32-7

RX(582) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(9), RX(32)  
RX(582) ET + 2 B + E + O + AC ==> EZ

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RX(95)      RCT    ET 636-61-3, B 67-56-1

STAGE(1)

RGT   D 7719-09-7 SOCl2  
CON   room temperature

STAGE(2)

RCT   E 106-95-6  
RGT   G 20667-12-3 Ag2O  
SOL   108-88-3 PhMe  
CON   room temperature

STAGE(3)

RGT   J 7529-22-8 Me-morpholineoxide  
CAT   20816-12-0 OsO4  
SOL   7732-18-5 Water, 109-99-9 THF  
CON   room temperature

STAGE(4)

RGT   K 7790-28-5 NaIO4  
SOL   7732-18-5 Water, 109-99-9 THF  
CON   room temperature

PRO   EU 441764-51-8

RX(96)      RCT    O 870-46-2, EU 441764-51-8

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PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H2  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(9) RCT AC 98-88-4, AD 609847-52-1

STAGE(1)  
SOL 110-86-1 Pyridine  
CON 25 minutes, room temperature

STAGE(2)  
SOL 7732-18-5 Water

PRO AE 609846-37-9

RX(32) RCT AE 609846-37-9

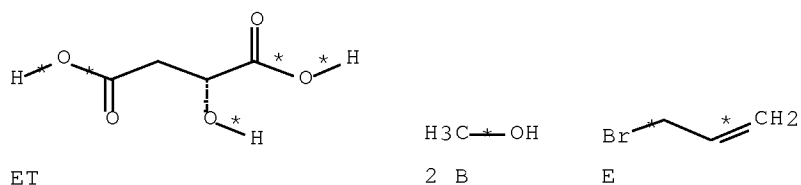
STAGE(1)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)  
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

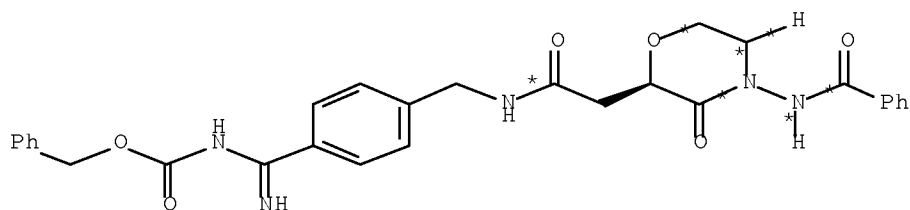
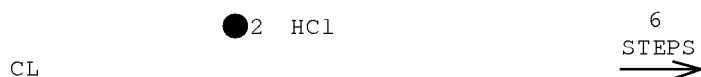
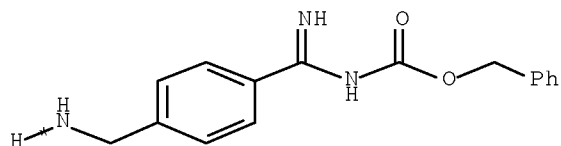
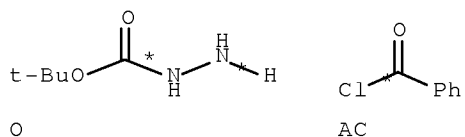
PRO BZ 609846-62-0

RX(583) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(9), RX(47)

RX(583) ET + 2 B + E + O + AC + CL ==>  
CQ



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CO  
YIELD 50%

RX(95)      RCT    ET 636-61-3, B 67-56-1

STAGE(1)

RGT   D 7719-09-7 SOCl<sub>2</sub>  
 CON   room temperature

STAGE(2)

RCT   E 106-95-6  
 RGT   G 20667-12-3 Ag<sub>2</sub>O  
 SOL   108-88-3 PhMe  
 CON   room temperature

STAGE(3)

RGT   J 7529-22-8 Me-morpholineoxide  
 CAT   20816-12-0 OsO<sub>4</sub>  
 SOL   7732-18-5 Water, 109-99-9 THF  
 CON   room temperature



STAGE(4)  
RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H2  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(9) RCT AC 98-88-4, AD 609847-52-1

STAGE(1)  
SOL 110-86-1 Pyridine  
CON 25 minutes, room temperature

STAGE(2)  
SOL 7732-18-5 Water

PRO AE 609846-37-9

RX(47) RCT AE 609846-37-9

STAGE(1)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

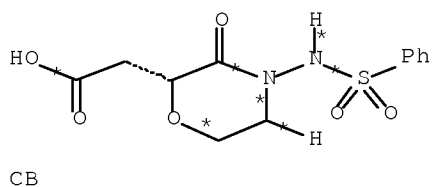
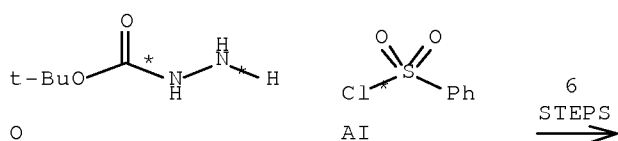
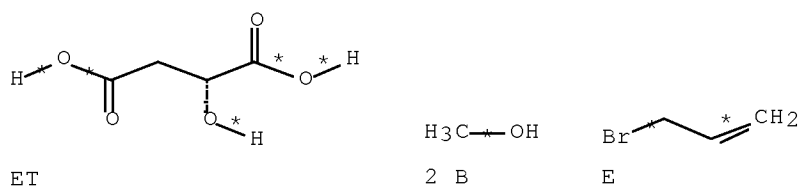
STAGE(2)  
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

STAGE(3)  
RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

PRO CQ 609846-77-7

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RX(584) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(11), RX(34)  
 RX(584) ET + 2 B + E + O + AI ==> CB



RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2  
 CON room temperature

STAGE(2)

RCT E 106-95-6  
 RGT G 20667-12-3 Ag2O  
 SOL 108-88-3 PhMe  
 CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
 CAT 20816-12-0 OsO4  
 SOL 7732-18-5 Water, 109-99-9 THF  
 CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4  
 SOL 7732-18-5 Water, 109-99-9 THF  
 CON room temperature

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PRO EU 441764-51-8

RX(96) RCT O ~~870-46-2~~, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H2  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(11) RCT AI 98-09-9, AD 609847-52-1  
PRO AJ 609846-39-1  
SOL 110-86-1 Pyridine  
CON 20 hours, room temperature

RX(34) RCT AJ 609846-39-1

STAGE(1)

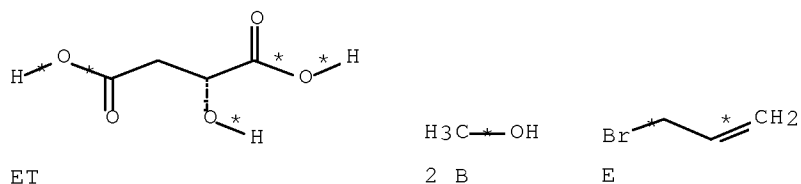
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)

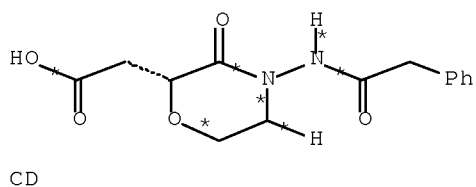
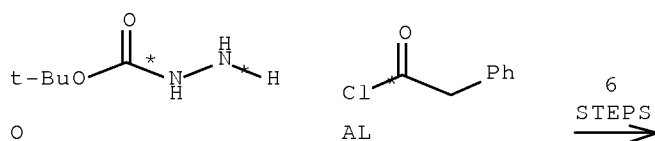
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

PRO CB ~~609846-64-2~~

RX(585) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(13), RX(36)  
RX(585) ET + 2 B + E + O + AL ==> CD



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RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl<sub>2</sub>

CON room temperature

STAGE(2)

RCT E 106-95-6

RGT G 20667-12-3 Ag<sub>2</sub>O

SOL 108-88-3 PhMe

CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide

CAT 20816-12-0 OsO<sub>4</sub>

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO<sub>4</sub>

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

PRO ES 609847-51-0

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C

SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0

RGT R 1333-74-0 H<sub>2</sub>

PRO AG 609847-50-9

CAT 7440-05-3 Pd

SOL 109-99-9 THF

CON 18 hours, room temperature

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RX(97) RCT AG 609847-50-9  
 PRO AD 609847-52-1  
 SOL 7732-18-5 Water  
 CON 7 hours, 60 deg C  
 NTE key intermediate

RX(13) RCT AL 103-80-0, AD 609847-52-1  
 PRO AM 609846-41-5  
 SOL 110-86-1 Pyridine  
 CON 29 hours, room temperature

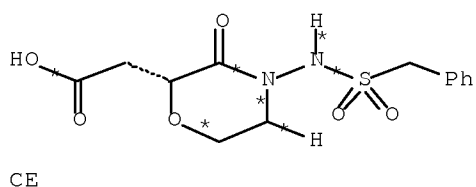
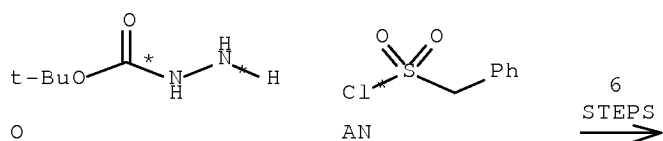
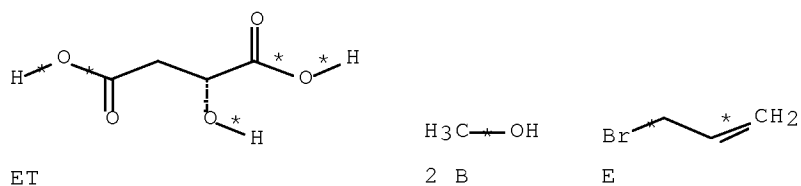
RX(36) RCT AM 609846-41-5

STAGE(1)  
 RGT BW 1310-65-2 LiOH  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON room temperature

STAGE(2)  
 RGT BX 7647-01-0 HCl  
 SOL 7732-18-5 Water  
 CON room temperature

PRO CD 609846-66-4

RX(586) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(14), RX(37)  
 RX(586) ET + 2 B + E + O + AN ==> CE



RX(95) RCT ET ~~636-61-3~~, B 67-56-1

STAGE(1)  
RGT D 7719-09-7 SOCl<sub>2</sub>  
CON room temperature

STAGE(2)  
RCT E 106-95-6  
RGT G 20667-12-3 Ag<sub>2</sub>O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)  
RGT K ~~7790-28-5~~ NaIO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O ~~870-46-2~~, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H<sub>2</sub>  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(14) RCT AN 1939-99-7, AD 609847-52-1  
PRO AO 609846-42-6  
SOL 110-86-1 Pyridine  
CON 24 hours, room temperature

RX(37) RCT AO 609846-42-6

STAGE(1)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

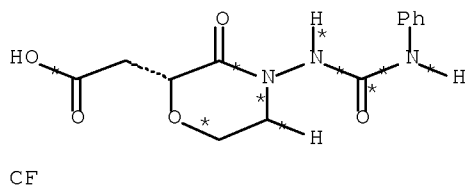
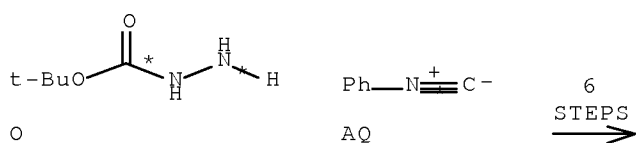
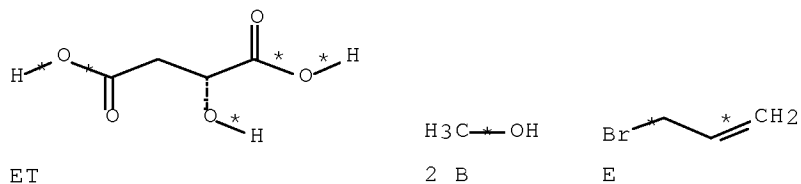
STAGE(2)

10/595943

RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

PRO CE 609846-67-5

RX(587) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(16), RX(38)  
RX(587) ET + 2 B + E + O + AQ ==> CF



RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2  
CON room temperature

STAGE(2)

RCT E 106-95-6  
RGT G 20667-12-3 Ag2O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF

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CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

PRO ES 609847-51-0

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C

SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0

RGT R 1333-74-0 H2

PRO AG 609847-50-9

CAT 7440-05-3 Pd

SOL 109-99-9 THF

CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9

PRO AD 609847-52-1

SOL 7732-18-5 Water

CON 7 hours, 60 deg C

NTE key intermediate

RX(16) RCT AQ 931-54-4, AD 609847-52-1

STAGE(1)

SOL 108-88-3 PhMe

CON 25 hours, room temperature

STAGE(2)

RGT B 67-56-1 MeOH

SOL 67-56-1 MeOH

CON 5 minutes, 40 deg C

PRO AR 609846-44-8

RX(38) RCT AR 609846-44-8

STAGE(1)

RGT BW 1310-65-2 LiOH

SOL 7732-18-5 Water, 67-56-1 MeOH

CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl

SOL 7732-18-5 Water

CON room temperature

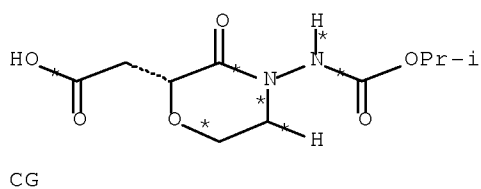
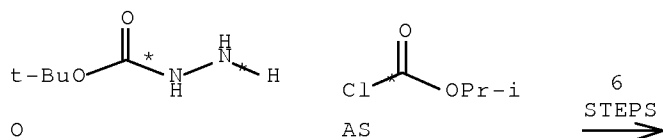
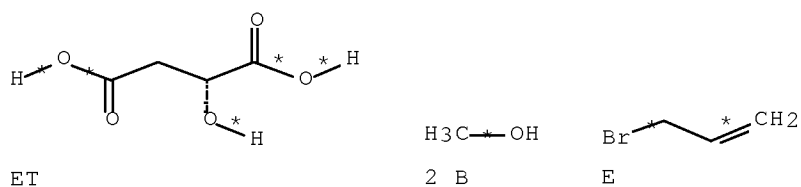
PRO CF 609846-68-6

RX(588) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(17), RX(39)

RX(588) ET + 2 B + E + O + AS ==> CG



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RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2  
CON room temperature

STAGE(2)

RCT E 106-95-6  
RGT G 20667-12-3 Ag2O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

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PRO ES 609847-51-0  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature -> 65 deg C  
 SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
 RGT R 1333-74-0 H2  
 PRO AG 609847-50-9  
 CAT 7440-05-3 Pd  
 SOL 109-99-9 THF  
 CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
 PRO AD 609847-52-1  
 SOL 7732-18-5 Water  
 CON 7 hours, 60 deg C  
 NTE key intermediate

RX(17) RCT AS 108-23-6, AD 609847-52-1  
 PRO AT 609846-45-9  
 SOL 108-88-3 PhMe, 110-86-1 Pyridine  
 CON SUBSTAGE(1) 0 deg C  
 SUBSTAGE(2) 4 hours

RX(39) RCT AT 609846-45-9

STAGE(1)

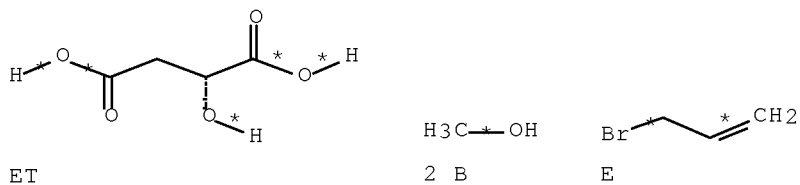
RGT BW 1310-65-2 LiOH  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON room temperature

STAGE(2)

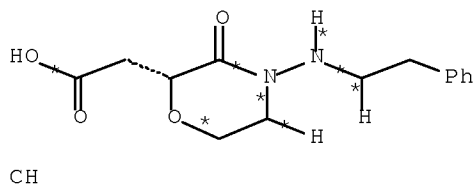
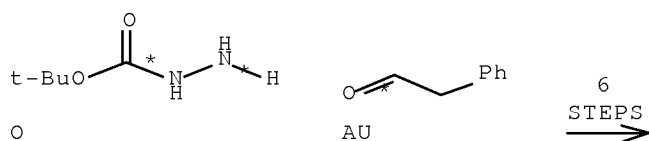
RGT BX 7647-01-0 HCl  
 SOL 7732-18-5 Water  
 CON room temperature

PRO CG 609846-69-7

RX(589) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(18), RX(40)  
 RX(589) ET + 2 B + E + O + AU ==> CH



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RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl<sub>2</sub>  
CON room temperature

STAGE(2)

RCT E 106-95-6  
RGT G 20667-12-3 Ag<sub>2</sub>O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H<sub>2</sub>  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

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RX(97) RCT AG 609847-50-9  
 PRO AD 609847-52-1  
 SOL 7732-18-5 Water  
 CON 7 hours, 60 deg C  
 NTE key intermediate

RX(18) RCT AU 122-78-1, AD 609847-52-1

STAGE(1)  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) overnight, 60 deg C

STAGE(2)  
 RGT R 1333-74-0 H2  
 CAT 7440-05-3 Pd  
 SOL 109-99-9 THF  
 CON 2 hours, room temperature

PRO AV 609846-46-0

RX(40) RCT AV 609846-46-0

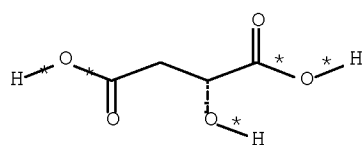
STAGE(1)  
 RGT BW 1310-65-2 LiOH  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON room temperature

STAGE(2)  
 RGT BX 7647-01-0 HCl  
 SOL 7732-18-5 Water  
 CON room temperature

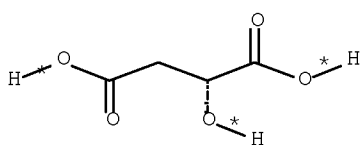
PRO CH 609846-70-0

RX(590) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(20), RX(41)

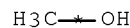
RX(590) 2 ET + 2 B + 2 E + 2 O + 3 AX ==>  
 CI



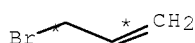
ET



ET

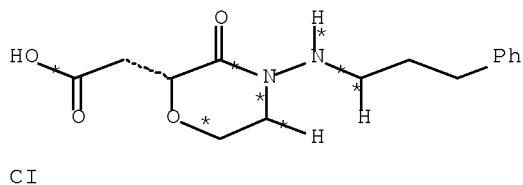
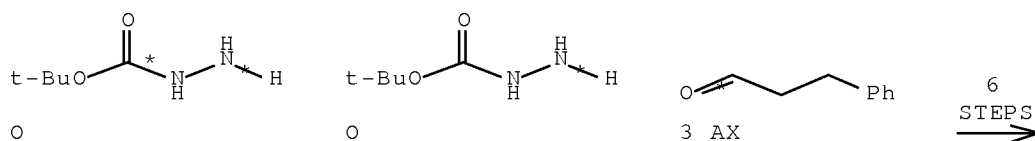


2 B



2 E

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RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl<sub>2</sub>  
CON room temperature

STAGE(2)

RCT E 106-95-6  
RGT G 20667-12-3 Ag<sub>2</sub>O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H<sub>2</sub>  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

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RX(97) RCT AG 609847-50-9  
 PRO AD 609847-52-1  
 SOL 7732-18-5 Water  
 CON 7 hours, 60 deg C  
 NTE key intermediate

RX(20) RCT AX 104-53-0, AD 609847-52-1

STAGE(1)  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) 24 hours, 70 deg C

STAGE(2)  
 RGT R 1333-74-0 H2  
 CAT 7440-05-3 Pd  
 SOL 109-99-9 THF  
 CON 70 minutes, room temperature

PRO AY 609846-48-2, AZ 609846-49-3

RX(41) RCT AY 609846-48-2

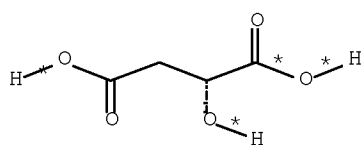
STAGE(1)  
 RGT BW 1310-65-2 LiOH  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON room temperature

STAGE(2)  
 RGT BX 7647-01-0 HCl  
 SOL 7732-18-5 Water  
 CON room temperature

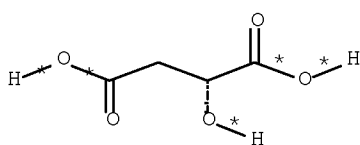
PRO CI 609846-71-1

RX(591) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(20), RX(43)

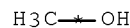
RX(591) 2 ET + 2 B + 2 E + 2 O + 3 AX ==>  
 CK



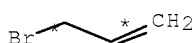
ET



ET

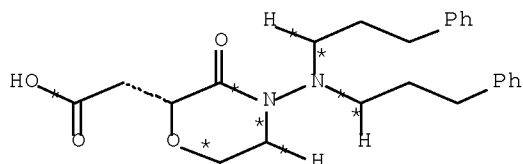
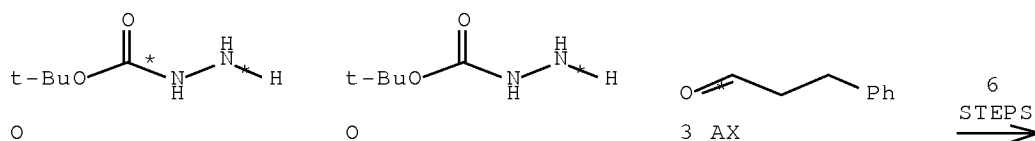


2 B



2 E

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RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl<sub>2</sub>

CON room temperature

STAGE(2)

RCT E 106-95-6

RGT G 20667-12-3 Ag<sub>2</sub>O

SOL 108-88-3 PhMe

CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide

CAT 20816-12-0 OsO<sub>4</sub>

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO<sub>4</sub>

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

PRO ES 609847-51-0

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C

SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0

RGT R 1333-74-0 H<sub>2</sub>

PRO AG 609847-50-9

CAT 7440-05-3 Pd

SOL 109-99-9 THF

CON 18 hours, room temperature

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RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(20) RCT AX 104-53-0, AD 609847-52-1

STAGE(1)  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) 24 hours, 70 deg C

STAGE(2)  
RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 70 minutes, room temperature

PRO AY 609846-48-2, AZ 609846-49-3

RX(43) RCT AZ 609846-49-3

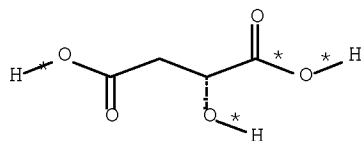
STAGE(1)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)  
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

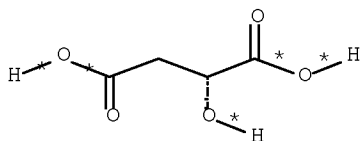
PRO CK 609846-73-3

RX(592) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(20), RX(60)

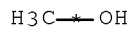
RX(592) 2 ET + 2 B + 2 E + 2 O + 3 AX + CL  
==> DD



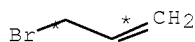
ET



ET



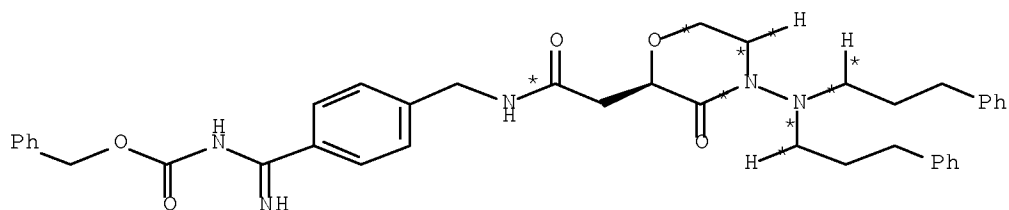
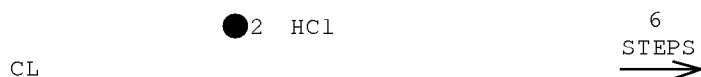
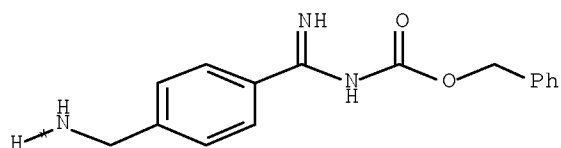
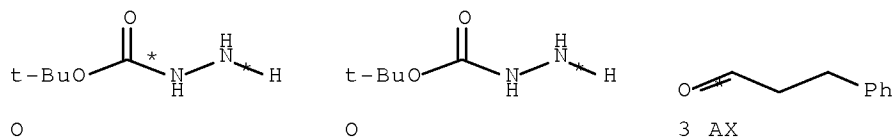
2 B



2 E



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DD  
YIELD 98%

RX(95)      RCT    ET 636-61-3, B 67-56-1

STAGE(1)

RGT   D 7719-09-7 SOCl<sub>2</sub>  
 CON   room temperature

STAGE(2)

RCT   E 106-95-6  
 RGT   G 20667-12-3 Ag<sub>2</sub>O  
 SOL   108-88-3 PhMe  
 CON   room temperature

STAGE(3)

RGT   J 7529-22-8 Me-morpholineoxide  
 CAT   20816-12-0 OsO<sub>4</sub>  
 SOL   7732-18-5 Water, 109-99-9 THF  
 CON   room temperature

STAGE(4)  
RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H2  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(20) RCT AX 104-53-0, AD 609847-52-1

STAGE(1)  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) 24 hours, 70 deg C

STAGE(2)  
RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 70 minutes, room temperature

PRO AY 609846-48-2, AZ 609846-49-3

RX(60) RCT AZ 609846-49-3

STAGE(1)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)  
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

STAGE(3)  
RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF

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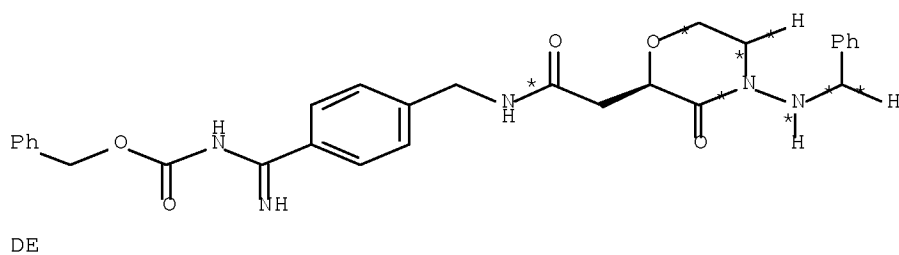
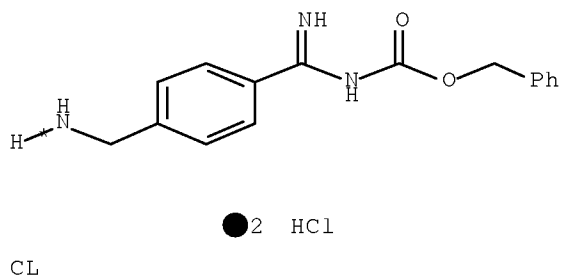
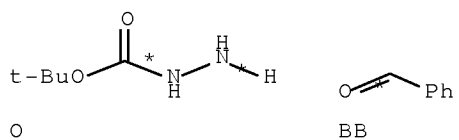
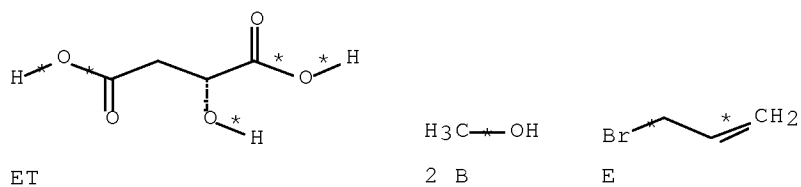
CON 100 minutes, room temperature

PRO DD 609846-90-4

RX(593) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(22), RX(61)

RX(593) ET + 2 B + E + O + BB + CL ==>

DE



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RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)  
RGT D 7719-09-7 SOC12  
CON room temperature

STAGE(2)  
RCT E 106-95-6  
RGT G 20667-12-3 Ag2O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)  
RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H2  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(22) RCT BB 100-52-7, AD 609847-52-1

STAGE(1)  
RGT BD 1125-88-8 PhCH(OMe)2  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 80 deg C  
SUBSTAGE(2) 2 days, 80 deg C

STAGE(2)  
RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 5 minutes, room temperature

PRO BC 609846-51-7

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RX(61) RCT BC 609846-51-7

STAGE(1)

RGT BW 1310-65-2 LiOH

SOL 7732-18-5 Water, 67-56-1 MeOH

CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl

SOL 7732-18-5 Water

CON room temperature

STAGE(3)

RCT CL 172348-75-3

RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2

SOL 68-12-2 DMF

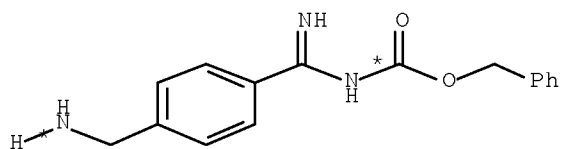
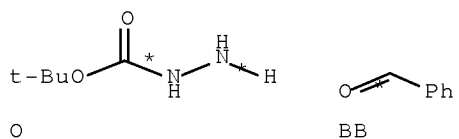
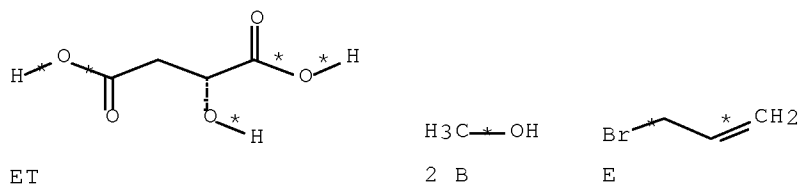
CON 100 minutes, room temperature

PRO DE 609846-91-5

RX(594) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(22), RX(86)

RX(594) ET + 2 B + E + O + BB + CL ==>

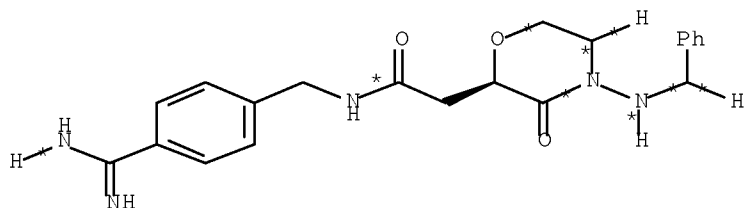
EF



● 2 HCl

6  
STEPS  
→

10/595943



EF  
YIELD 100%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl<sub>2</sub>  
CON room temperature

STAGE(2)

RCT E 106-95-6  
RGT G 20667-12-3 Ag<sub>2</sub>O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H<sub>2</sub>  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water

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CON 7 hours, 60 deg C  
NTE key intermediate

RX(22) RCT BB 100-52-7, AD 609847-52-1

STAGE(1)

RGT BD 1125-88-8 PhCH(OMe)2  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 80 deg C  
SUBSTAGE(2) 2 days, 80 deg C

STAGE(2)

RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 5 minutes, room temperature

PRO BC 609846-51-7

RX(86) RCT BC 609846-51-7

STAGE(1)

RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

STAGE(3)

RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

STAGE(4)

RGT EG 1493-13-6 F3CSO2H, EH 100-66-3 PhOMe  
SOL 75-09-2 CH2Cl2  
CON 15 minutes, 0 deg C

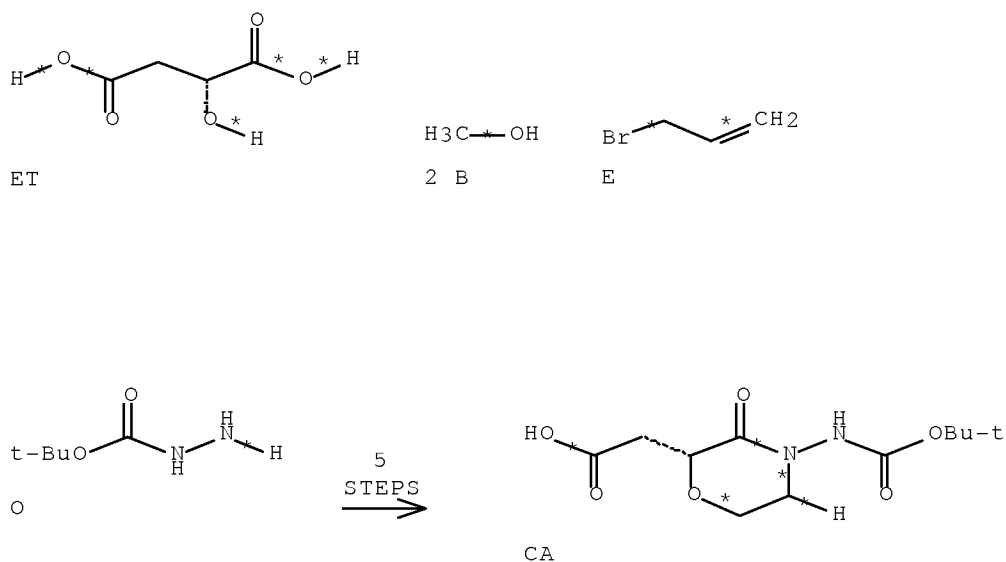
STAGE(5)

RGT EI 121-44-8 Et3N  
CON neutralized

PRO EF 609847-33-8

RX(595) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(10), RX(33)  
RX(595) ET + 2 B + E + O ==> CA

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RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOC12

CON room temperature

STAGE(2)

RCT E 106-95-6

RGT G 20667-12-3 Ag2O

SOL 108-88-3 PhMe

CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide

CAT 20816-12-0 OsO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

PRO ES 609847-51-0

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C

SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0

RGT R 1333-74-0 H2

PRO AG 609847-50-9

CAT 7440-05-3 Pd

SOL 109-99-9 THF



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CON 18 hours, room temperature

RX(10) RCT AG 609847-50-9  
 PRO AH 609846-38-0  
 SOL 108-88-3 PhMe  
 CON 3 days, reflux

RX(33) RCT AH 609846-38-0

STAGE(1)

RGT BW 1310-65-2 LiOH  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON room temperature

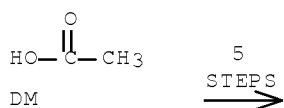
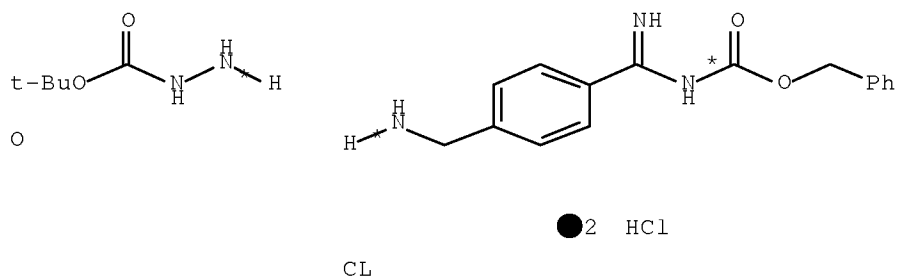
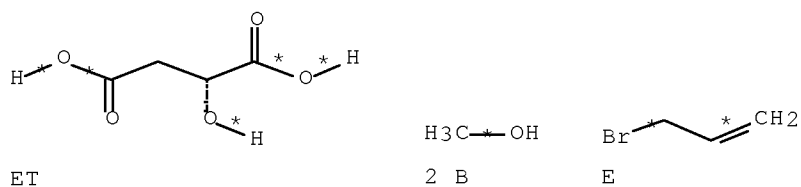
STAGE(2)

RGT BX 7647-01-0 HCl  
 SOL 7732-18-5 Water  
 CON room temperature

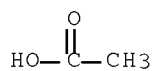
PRO CA 609846-63-1

RX(596) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(10), RX(73)

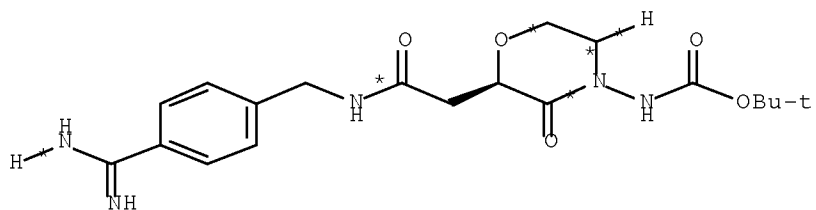
RX(596) ET + 2 B + E + O + CL + DM ==>  
 DS



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DS: CM 1  
YIELD 39%



DS: CM 2  
YIELD 39%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2  
CON room temperature

STAGE(2)

RCT E 106-95-6  
RGT G 20667-12-3 Ag2O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H2  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(10) RCT AG 609847-50-9  
PRO AH 609846-38-0  
SOL 108-88-3 PhMe  
CON 3 days, reflux

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RX(73) RCT AH 609846-38-0

STAGE(1)

RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

STAGE(3)

RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

STAGE(4)

RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 7732-18-5 Water, 64-17-5 EtOH  
CON 45 minutes, room temperature

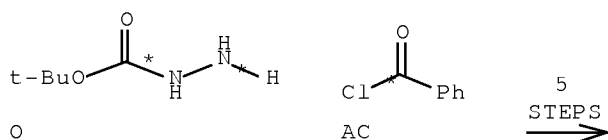
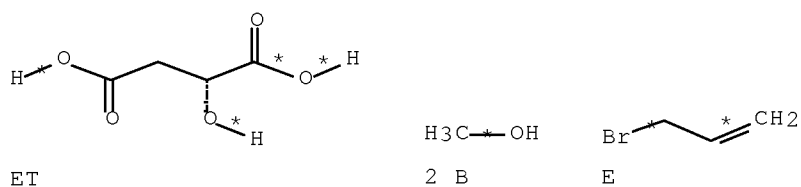
STAGE(5)

RCT DM 64-19-7  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

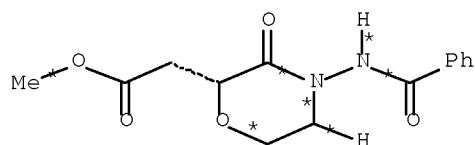
PRO DS 609847-08-7

RX(597) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(9)

RX(597) ET + 2 B + E + O + AC ==> AE



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AE  
YIELD 97%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl<sub>2</sub>  
CON room temperature

STAGE(2)

RCT E 106-95-6  
RGT G 20667-12-3 Ag<sub>2</sub>O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H<sub>2</sub>  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(9) RCT AC 98-88-4, AD 609847-52-1

STAGE(1)

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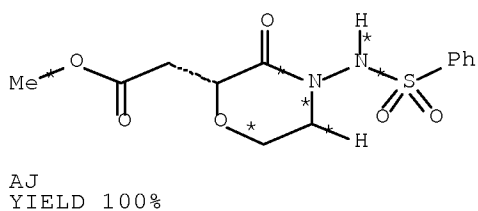
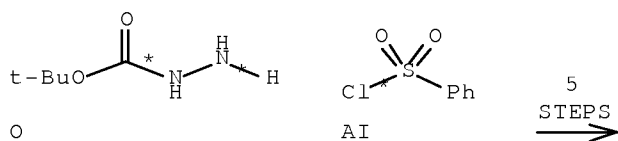
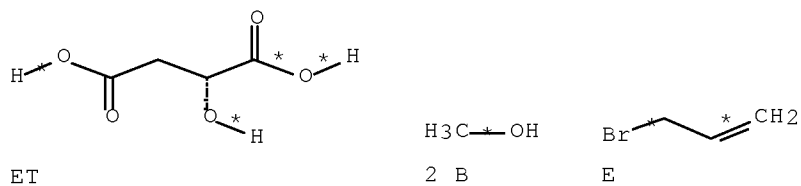
SOL 110-86-1 Pyridine  
CON 25 minutes, room temperature

STAGE(2)

SOL 7732-18-5 Water

PRO AE 609846-37-9

RX(598) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(11)  
RX(598) ET + 2 B + E + O + AI ==> AJ



RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2  
CON room temperature

STAGE(2)

RCT E 106-95-6  
RGT G 20667-12-3 Ag2O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)

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RGT J 7529-22-8 Me-morpholineoxide  
 CAT 20816-12-0 OsO4  
 SOL 7732-18-5 Water, 109-99-9 THF  
 CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4  
 SOL 7732-18-5 Water, 109-99-9 THF  
 CON room temperature

PRO EU 441764-51-8

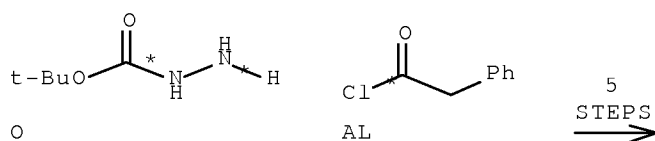
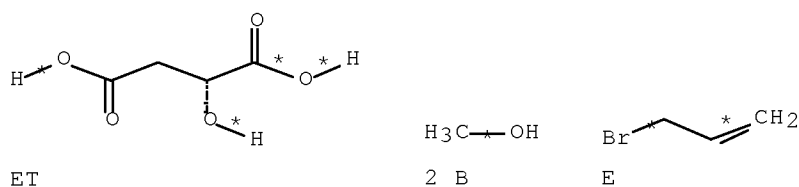
RX(96) RCT O 870-46-2, EU 441764-51-8  
 PRO ES 609847-51-0  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature -> 65 deg C  
 SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
 RGT R 1333-74-0 H2  
 PRO AG 609847-50-9  
 CAT 7440-05-3 Pd  
 SOL 109-99-9 THF  
 CON 18 hours, room temperature

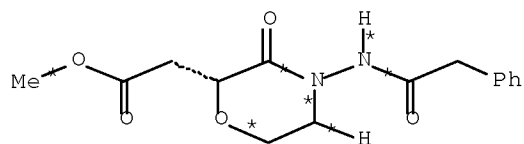
RX(97) RCT AG 609847-50-9  
 PRO AD 609847-52-1  
 SOL 7732-18-5 Water  
 CON 7 hours, 60 deg C  
 NTE key intermediate

RX(11) RCT AI 98-09-9, AD 609847-52-1  
 PRO AJ 609846-39-1  
 SOL 110-86-1 Pyridine  
 CON 20 hours, room temperature

RX(599) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(13)  
 RX(599) ET + 2 B + E + O + AL ==> AM



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AM  
YIELD 49%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl<sub>2</sub>

CON room temperature

STAGE(2)

RCT E 106-95-6

RGT G 20667-12-3 Ag<sub>2</sub>O

SOL 108-88-3 PhMe

CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide

CAT 20816-12-0 OsO<sub>4</sub>

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO<sub>4</sub>

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

PRO ES 609847-51-0

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C

SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0

RGT R 1333-74-0 H<sub>2</sub>

PRO AG 609847-50-9

CAT 7440-05-3 Pd

SOL 109-99-9 THF

CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9

PRO AD 609847-52-1

SOL 7732-18-5 Water

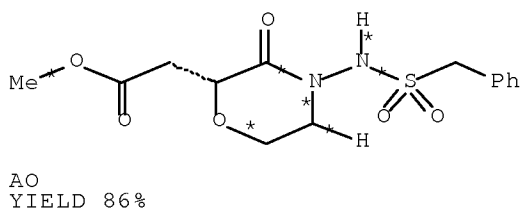
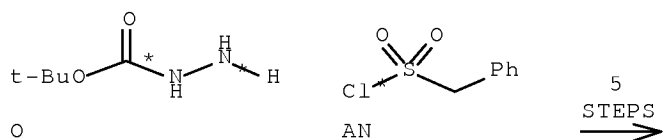
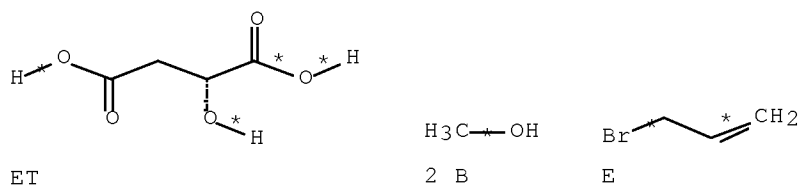
CON 7 hours, 60 deg C

NTE key intermediate

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RX(13) RCT AL 103-80-0, AD 609847-52-1  
 PRO AM 609846-41-5  
 SOL 110-86-1 Pyridine  
 CON 29 hours, room temperature

RX(600) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(14)  
 RX(600) ET + 2 B + E + O + AN ==> AO



RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2  
 CON room temperature

STAGE(2)

RCT E 106-95-6  
 RGT G 20667-12-3 Ag2O  
 SOL 108-88-3 PhMe  
 CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
 CAT 20816-12-0 OsO4  
 SOL 7732-18-5 Water, 109-99-9 THF



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CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

PRO ES 609847-51-0

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C

SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0

RGT R 1333-74-0 H2

PRO AG 609847-50-9

CAT 7440-05-3 Pd

SOL 109-99-9 THF

CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9

PRO AD 609847-52-1

SOL 7732-18-5 Water

CON 7 hours, 60 deg C

NTE key intermediate

RX(14) RCT AN 1939-99-7, AD 609847-52-1

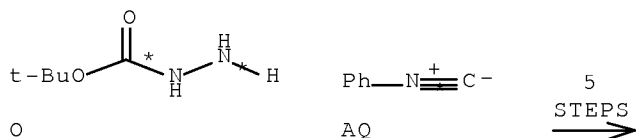
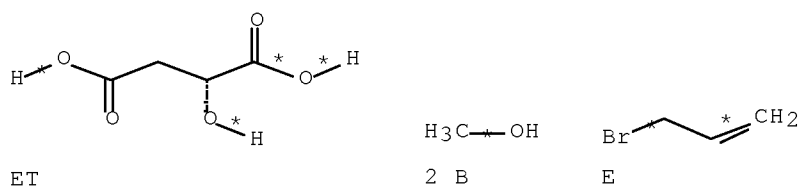
PRO AO 609846-42-6

SOL 110-86-1 Pyridine

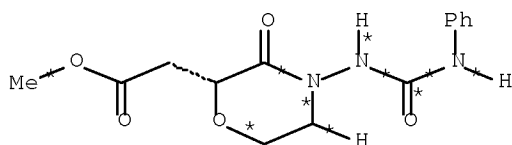
CON 24 hours, room temperature

RX(601) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(16)

RX(601) ET + 2 B + E + O + AQ ==> AR



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AR  
YIELD 100%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl<sub>2</sub>  
CON room temperature

STAGE(2)

RCT E 106-95-6  
RGT G 20667-12-3 Ag<sub>2</sub>O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H<sub>2</sub>  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(16) RCT AQ 931-54-4, AD 609847-52-1

STAGE(1)

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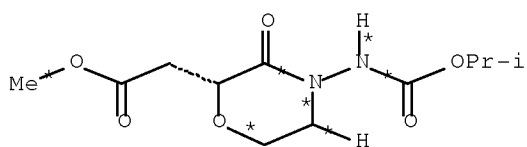
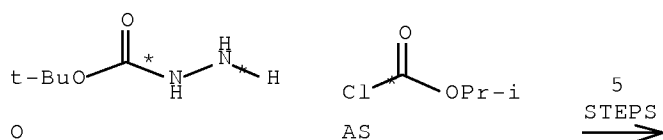
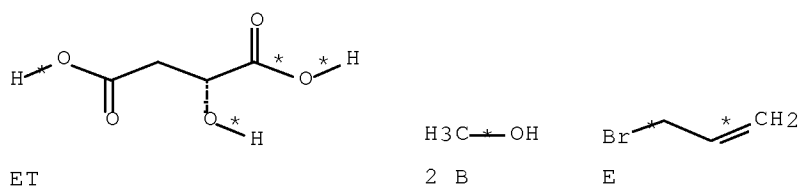
SOL 108-88-3 PhMe  
CON 25 hours, room temperature

STAGE(2)

RGT B 67-56-1 MeOH  
SOL 67-56-1 MeOH  
CON 5 minutes, 40 deg C

PRO AR 609846-44-8

RX(602) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(17)  
RX(602) ET + 2 B + E + O + AS ==> AT



YIELD 93%

RX(95)      RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2  
CON room temperature

STAGE(2)

RCT E 106-95-6  
RGT G 20667-12-3 Ag2O  
SOL 108-88-3 PhMe  
CON room temperature

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STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

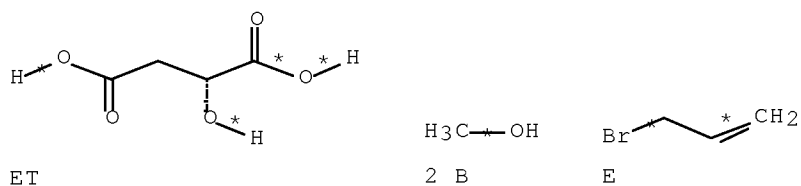
RX(96) RCT O 870-46-2, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H2  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

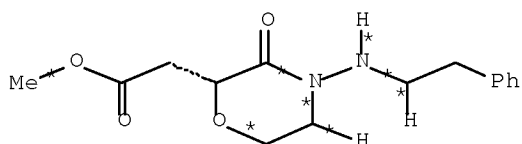
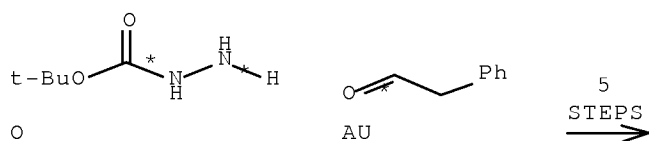
RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(17) RCT AS 108-23-6, AD 609847-52-1  
PRO AT 609846-45-9  
SOL 108-88-3 PhMe, 110-86-1 Pyridine  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 4 hours

RX(603) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(18)  
RX(603) ET + 2 B + E + O + AU ==> AV



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AV  
YIELD 100%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOC12

CON room temperature

STAGE(2)

RCT E 106-95-6

RGT G 20667-12-3 Ag2O

SOL 108-88-3 PhMe

CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide

CAT 20816-12-0 OsO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

PRO ES 609847-51-0

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C

SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0

RGT R 1333-74-0 H2

PRO AG 609847-50-9

CAT 7440-05-3 Pd

SOL 109-99-9 THF

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CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
 PRO AD 609847-52-1  
 SOL 7732-18-5 Water  
 CON 7 hours, 60 deg C  
 NTE key intermediate

RX(18) RCT AU 122-78-1, AD 609847-52-1

STAGE(1)

SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) overnight, 60 deg C

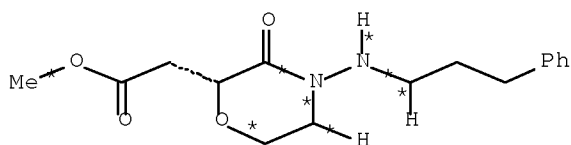
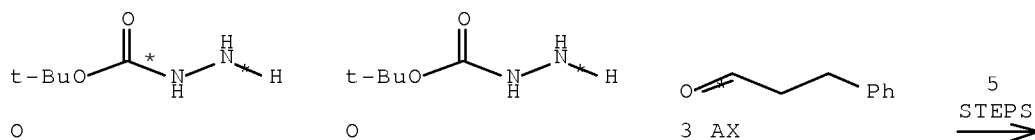
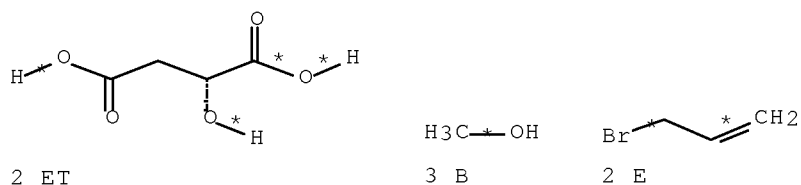
STAGE(2)

RGT R 1333-74-0 H2  
 CAT 7440-05-3 Pd  
 SOL 109-99-9 THF  
 CON 2 hours, room temperature

PRO AV 609846-46-0

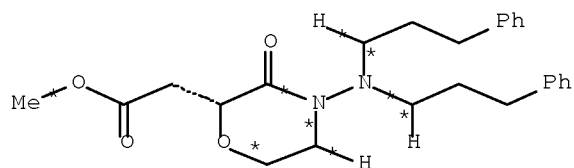
RX(604) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(20)

RX(604) 2 ET + 3 B + 2 E + 2 O + 3 AX ==>  
 AY + AZ



AY  
 YIELD 55%

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AZ  
YIELD 37%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl<sub>2</sub>  
CON room temperature

STAGE(2)

RCT E 106-95-6  
RGT G 20667-12-3 Ag<sub>2</sub>O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO<sub>4</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H<sub>2</sub>  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

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RX(20) RCT AX 104-53-0, AD 609847-52-1

STAGE(1)

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 24 hours, 70 deg C

STAGE(2)

RGT R 1333-74-0 H2

CAT 7440-05-3 Pd

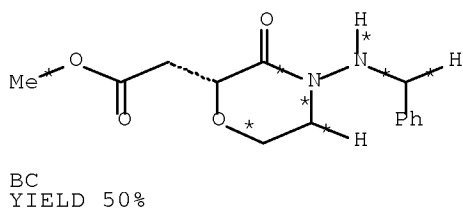
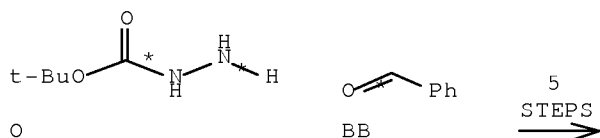
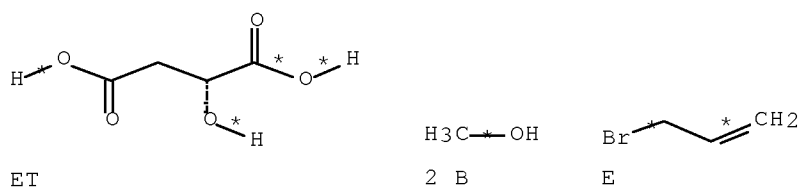
SOL 109-99-9 THF

CON 70 minutes, room temperature

PRO AY 609846-48-2, AZ 609846-49-3

RX(605) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(22)

RX(605) ET + 2 B + E + O + BB ==> BC



RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2



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CON room temperature

STAGE(2)

RCT E 106-95-6  
RGT G 20667-12-3 Ag2O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H2  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(22) RCT BB 100-52-7, AD 609847-52-1

STAGE(1)

RGT BD 1125-88-8 PhCH(OMe)2  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 80 deg C  
SUBSTAGE(2) 2 days, 80 deg C

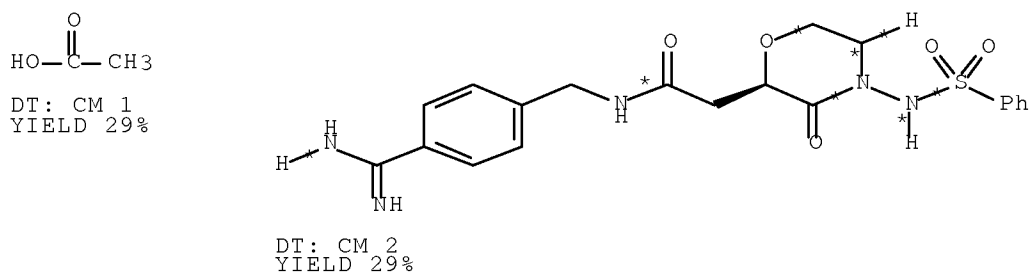
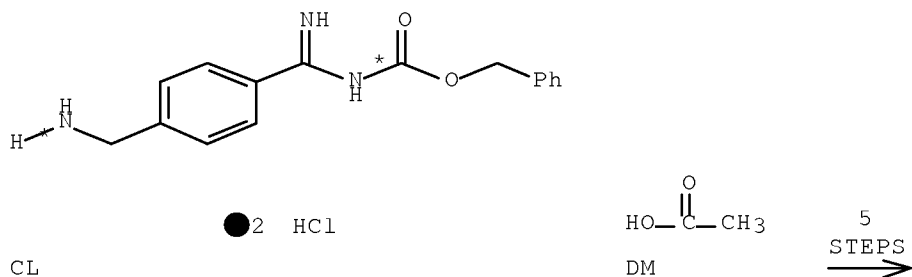
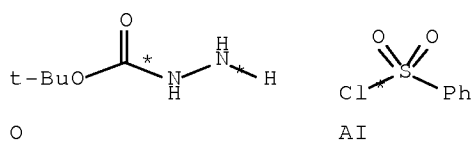
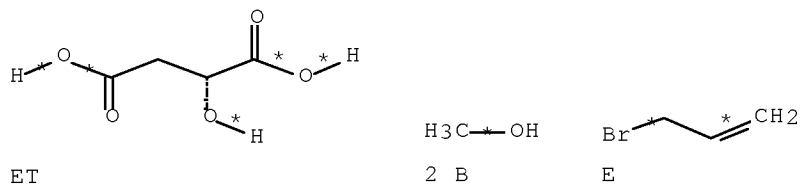
STAGE(2)

RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 5 minutes, room temperature

PRO BC 609846-51-7

RX(606) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(74)  
RX(606) ET + 2 B + E + O + AI + CL + DM ==>  
DT

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RX(95)      RCT   ET 636-61-3, B 67-56-1

STAGE(1)

RGT   D 7719-09-7 SOCl2

CON   room temperature

STAGE(2)  
RCT E 106-95-6  
RGT G 20667-12-3 Ag2O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)  
RGT K ~~7790-28-5~~ NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O ~~870-46-2~~, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H2  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(74) RCT AI 98-09-9, AD 609847-52-1

STAGE(1)  
SOL 110-86-1 Pyridine  
CON 20 hours, room temperature

STAGE(2)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(3)  
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

STAGE(4)  
RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2

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SOL 68-12-2 DMF  
CON 100 minutes, room temperature

STAGE(5)

RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 7732-18-5 Water, 64-17-5 EtOH  
CON 80 minutes, room temperature

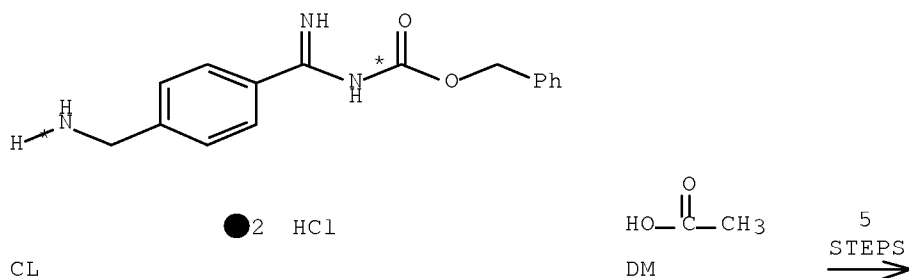
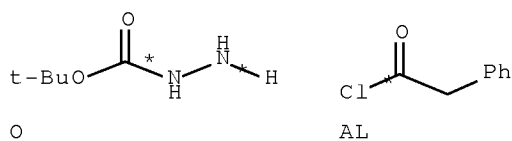
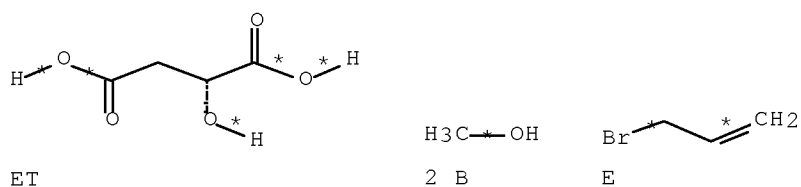
STAGE(6)

RCT DM 64-19-7  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

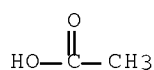
PRO DT 609847-10-1

RX(607) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(76)

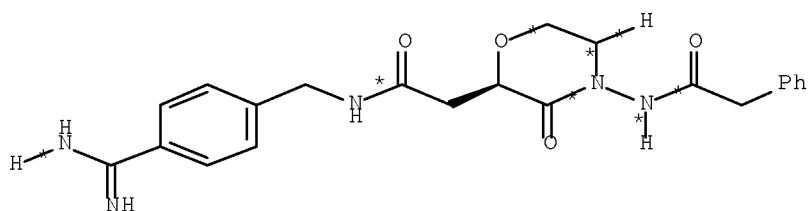
RX(607) ET + 2 B + E + O + AL + CL + DM ==>  
DV



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DV: CM 1  
YIELD 26%



DV: CM 2  
YIELD 26%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2  
CON room temperature

STAGE(2)

RCT E 106-95-6  
RGT G 20667-12-3 Ag2O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H2  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(76) RCT AL 103-80-0, AD 609847-52-1

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STAGE(1)

SOL 110-86-1 Pyridine  
CON 29 hours, room temperature

STAGE(2)

RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(3)

RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

STAGE(4)

RCT CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

STAGE(5)

RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 7732-18-5 Water, 64-17-5 EtOH  
CON 60 minutes, room temperature

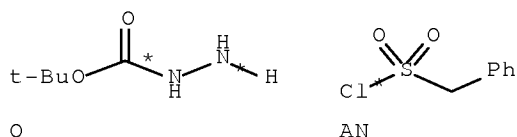
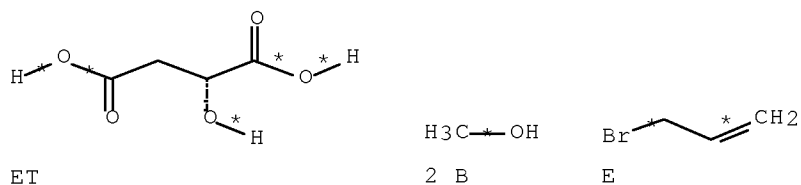
STAGE(6)

RCT DM 64-19-7  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

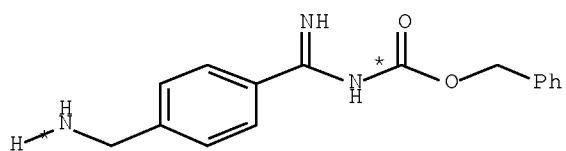
PRO DV 609847-14-5

RX(608) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(77)

RX(608) ET + 2 B + E + O + AN + CL + DM ==>  
DW

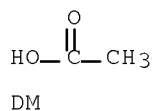


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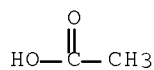


CL

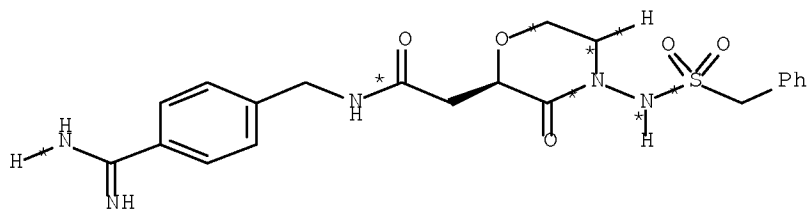
●2 HCl



5  
STEPS  
→



DW: CM 1  
YIELD 43%



DW: CM 2  
YIELD 43%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOC12  
CON room temperature

STAGE(2)

RCT E 106-95-6  
RGT G 20667-12-3 Ag2O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

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```
RX(96)  RCT  O 870-46-2, EU 441764-51-8
        PRO  ES 609847-51-0
        SOL  108-88-3 PhMe
        CON  SUBSTAGE(1) room temperature -> 65 deg C
           SUBSTAGE(2) overnight, 65 deg C

RX(94)  RCT  ES 609847-51-0
        RGT  R 1333-74-0 H2
        PRO  AG 609847-50-9
        CAT  7440-05-3 Pd
        SOL  109-99-9 THF
        CON  18 hours, room temperature

RX(97)  RCT  AG 609847-50-9
        PRO  AD 609847-52-1
        SOL  7732-18-5 Water
        CON  7 hours, 60 deg C
        NTE  key intermediate

RX(77)  RCT  AN 1939-99-7, AD 609847-52-1

        STAGE(1)
          SOL  110-86-1 Pyridine
          CON  24 hours, room temperature

        STAGE(2)
          RGT  BW 1310-65-2 LiOH
          SOL  7732-18-5 Water, 67-56-1 MeOH
          CON  room temperature

        STAGE(3)
          RGT  BX 7647-01-0 HCl
          SOL  7732-18-5 Water
          CON  room temperature

        STAGE(4)
          RCT  CL 172348-75-3
          RGT  CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
              1-[bis(dimethylamino)methylene]-, 3-oxide,
              hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
          SOL  68-12-2 DMF
          CON  100 minutes, room temperature

        STAGE(5)
          RGT  R 1333-74-0 H2
          CAT  7440-05-3 Pd
          SOL  7732-18-5 Water, 64-17-5 EtOH
          CON  31 hours, room temperature

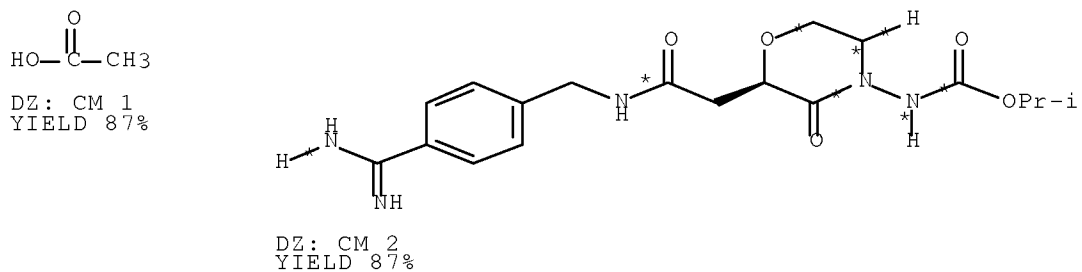
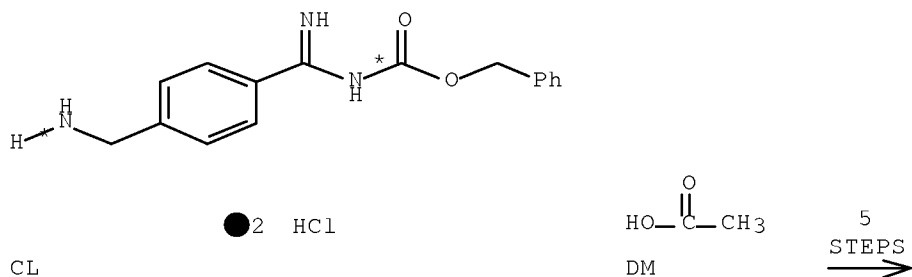
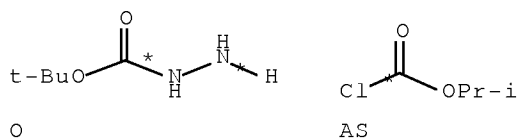
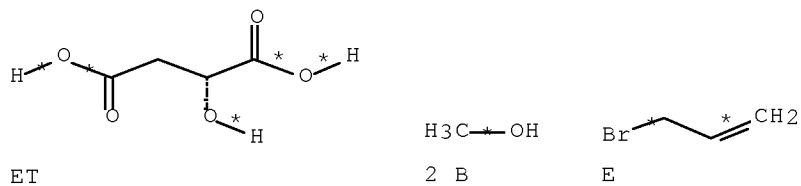
        STAGE(6)
          RCT  DM 64-19-7
          SOL  7732-18-5 Water, 67-56-1 MeOH
          CON  room temperature

        PRO  DW 609847-16-7

RX(609) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(80)
RX(609)  ET  + 2 B + E + O + AS + CL + DM ==>
        DZ
```



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RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2

CON room temperature

## STAGE(2)

RCT E 106-95-6  
 RGT G 20667-12-3 Ag2O  
 SOL 108-88-3 PhMe  
 CON room temperature

## STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
 CAT 20816-12-0 OsO4  
 SOL 7732-18-5 Water, 109-99-9 THF  
 CON room temperature

## STAGE(4)

RGT K ~~7790-28-5~~ NaIO4  
 SOL 7732-18-5 Water, 109-99-9 THF  
 CON room temperature

PRO EU 441764-51-8

RX(96) RCT O ~~870-46-2~~, EU 441764-51-8  
 PRO ES 609847-51-0  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature -> 65 deg C  
 SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
 RGT R 1333-74-0 H2  
 PRO AG 609847-50-9  
 CAT 7440-05-3 Pd  
 SOL 109-99-9 THF  
 CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
 PRO AD 609847-52-1  
 SOL 7732-18-5 Water  
 CON 7 hours, 60 deg C  
 NTE key intermediate

RX(80) RCT AS 108-23-6, AD 609847-52-1

## STAGE(1)

SOL 108-88-3 PhMe, 110-86-1 Pyridine  
 CON SUBSTAGE(1) 0 deg C  
 SUBSTAGE(2) 4 hours

## STAGE(2)

RGT BW 1310-65-2 LiOH  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON room temperature

## STAGE(3)

RGT BX 7647-01-0 HCl  
 SOL 7732-18-5 Water  
 CON room temperature

## STAGE(4)

RCT CL 172348-75-3  
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
 1-[bis(dimethylamino)methylene]-, 3-oxide,

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hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
 SOL 68-12-2 DMF  
 CON 100 minutes, room temperature

STAGE(5)

RGT R 1333-74-0 H2  
 CAT 7440-05-3 Pd  
 SOL 7732-18-5 Water, 64-17-5 EtOH  
 CON 1 hour, room temperature

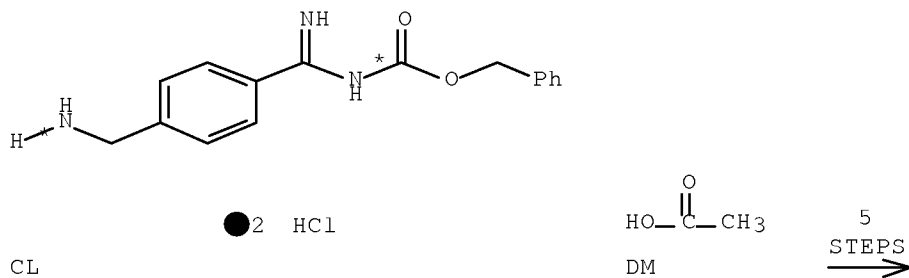
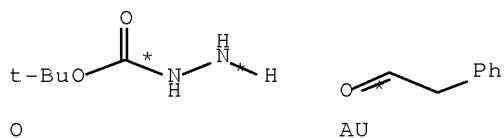
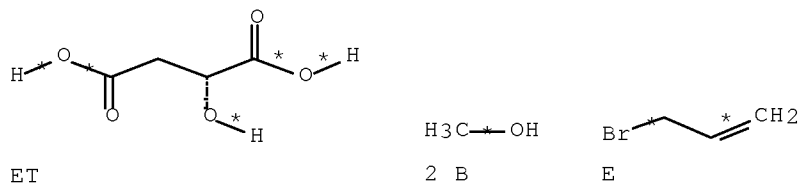
STAGE(6)

RCT DM 64-19-7  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON room temperature

PRO DZ 609847-22-5

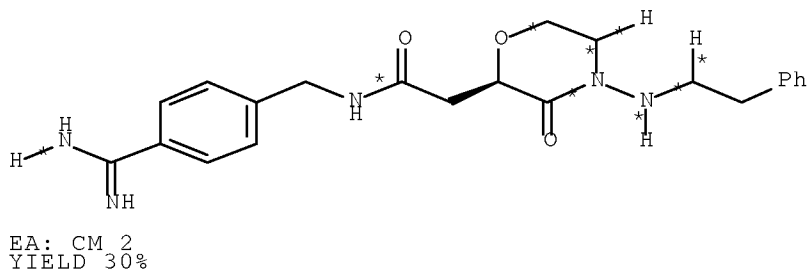
RX(610) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(81)

RX(610) ET + 2 B + E + O + AU + CL + DM ==>  
 EA



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$\text{HO}-\overset{\text{O}}{\parallel}{\text{C}}-\text{CH}_3$   
 EA: CM 1  
 YIELD 30%



RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl<sub>2</sub>  
 CON room temperature

STAGE(2)

RCT E 106-95-6  
 RGT G 20667-12-3 Ag<sub>2</sub>O  
 SOL 108-88-3 PhMe  
 CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
 CAT 20816-12-0 OsO<sub>4</sub>  
 SOL 7732-18-5 Water, 109-99-9 THF  
 CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO<sub>4</sub>  
 SOL 7732-18-5 Water, 109-99-9 THF  
 CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8  
 PRO ES 609847-51-0  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature -> 65 deg C  
 SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
 RGT R 1333-74-0 H<sub>2</sub>  
 PRO AG 609847-50-9  
 CAT 7440-05-3 Pd  
 SOL 109-99-9 THF  
 CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
 PRO AD 609847-52-1  
 SOL 7732-18-5 Water  
 CON 7 hours, 60 deg C  
 NTE key intermediate

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RX(81) RCT AU 122-78-1, AD 609847-52-1

STAGE(1)

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) overnight, 60 deg C

STAGE(2)

RGT R 1333-74-0 H2

CAT 7440-05-3 Pd

SOL 109-99-9 THF

CON 2 hours, room temperature

STAGE(3)

RGT BW 1310-65-2 LiOH

SOL 7732-18-5 Water, 67-56-1 MeOH

CON room temperature

STAGE(4)

RGT BX 7647-01-0 HCl

SOL 7732-18-5 Water

CON room temperature

STAGE(5)

RCT CL 172348-75-3

RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2

SOL 68-12-2 DMF

CON 100 minutes, room temperature

STAGE(6)

RGT R 1333-74-0 H2

CAT 7440-05-3 Pd

SOL 7732-18-5 Water, 64-17-5 EtOH

CON 80 minutes, room temperature

STAGE(7)

RCT DM 64-19-7

SOL 7732-18-5 Water, 67-56-1 MeOH

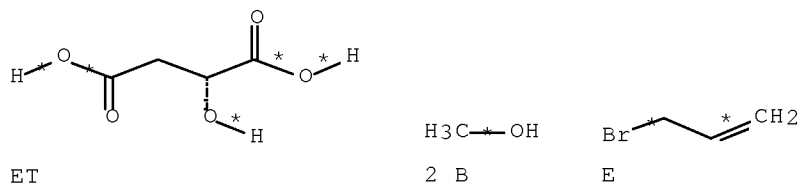
CON room temperature

PRO EA 609847-24-7

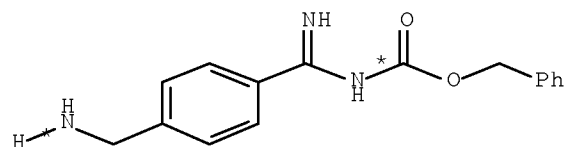
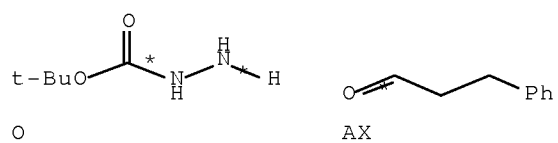
RX(611) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(83)

RX(611) ET + 2 B + E + O + AX + CL + DM ==>

EC

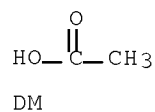


10/595943

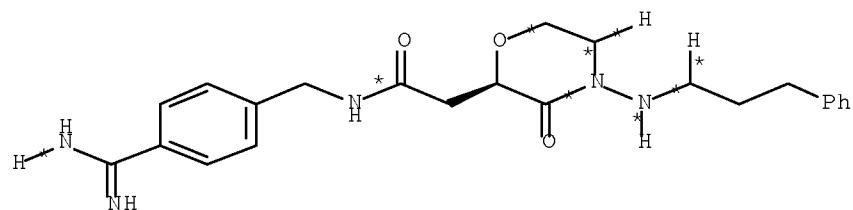
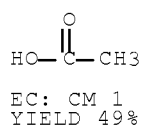


CL

● 2 HCl



5  
STEPS  
→



EC: CM 2  
YIELD 49%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOC12  
CON room temperature

STAGE(2)

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RCT E 106-95-6  
RGT G 20667-12-3 Ag2O  
SOL 108-88-3 PhMe  
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(4)

RGT K ~~7790-28-5~~ NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O ~~870-46-2~~, EU 441764-51-8  
PRO ES 609847-51-0  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H2  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(83) RCT AX 104-53-0, AD 609847-52-1

STAGE(1)

SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) 24 hours, 70 deg C

STAGE(2)

RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 70 minutes, room temperature

STAGE(3)

RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(4)

RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

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STAGE(5)

RCT CL 172348-75-3  
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
 1-[bis(dimethylamino)methylene]-, 3-oxide,  
 hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
 SOL 68-12-2 DMF  
 CON 100 minutes, room temperature

STAGE(6)

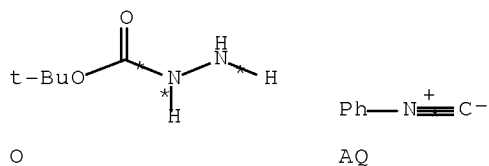
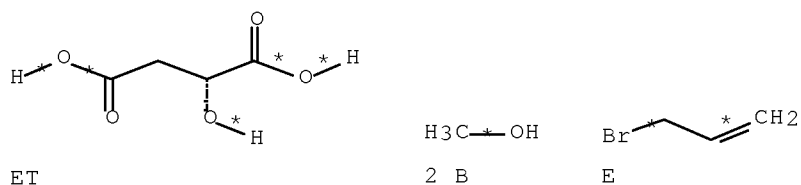
RGT R 1333-74-0 H2  
 CAT 7440-05-3 Pd  
 SOL 7732-18-5 Water, 64-17-5 EtOH  
 CON 2 hours, room temperature

STAGE(7)

RCT DM 64-19-7  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON room temperature

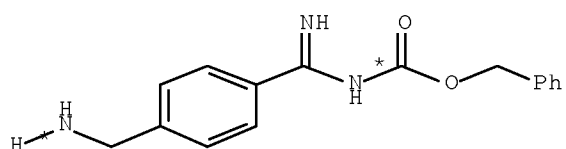
PRO EC 609847-28-1

RX(612) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(16), RX(38),  
 RX(54), RX(79)  
 RX(612) ET + 2 B + E + O + AQ + CL + DM ==>  
 DY



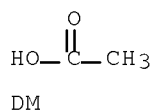


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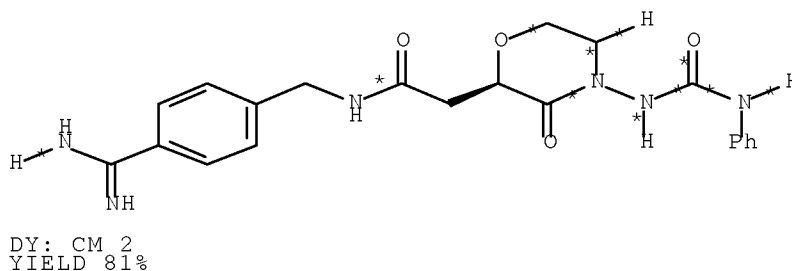
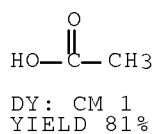


CL

●2 HCl



8  
STEPS  
→



RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOC12

CON room temperature

STAGE(2)

RCT E 106-95-6

RGT G 20667-12-3 Ag2O

SOL 108-88-3 PhMe

CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide

CAT 20816-12-0 OsO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

PRO ES 609847-51-0

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C

SUBSTAGE(2) overnight, 65 deg C

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RX(94) RCT ES 609847-51-0  
RGT R 1333-74-0 H2  
PRO AG 609847-50-9  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9  
PRO AD 609847-52-1  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(16) RCT AQ 931-54-4, AD 609847-52-1

STAGE(1)  
SOL 108-88-3 PhMe  
CON 25 hours, room temperature

STAGE(2)  
RGT B 67-56-1 MeOH  
SOL 67-56-1 MeOH  
CON 5 minutes, 40 deg C

PRO AR 609846-44-8

RX(38) RCT AR 609846-44-8

STAGE(1)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)  
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

PRO CF 609846-68-6

RX(54) RCT CF 609846-68-6, CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
PRO CX 609846-84-6  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

RX(79) RCT CX 609846-84-6

STAGE(1)  
RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 7732-18-5 Water, 64-17-5 EtOH, 109-99-9 THF  
CON 2 hours, room temperature

STAGE(2)  
RCT DM 64-19-7  
SOL 7732-18-5 Water, 67-56-1 MeOH

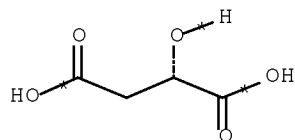
10/595943

CON room temperature

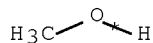
PRO DY 609847-20-3

RX(613) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(7),  
RX(44), RX(69)

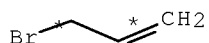
RX(613) A + 2 B + E + O + U + CL + DM ==>  
DN



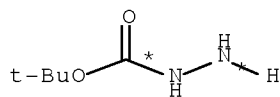
A



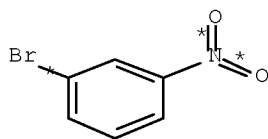
2 B



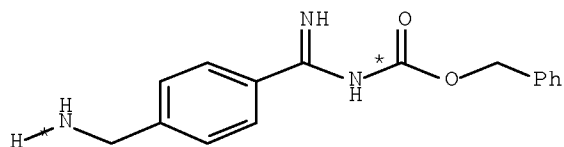
E



O

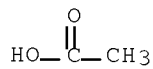


U



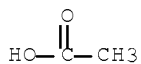
CL

● 2 HCl



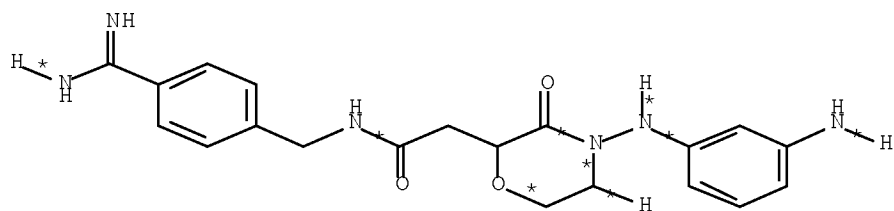
DM

9  
STEPS  
➔



DN: CM 1  
YIELD 48%

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DN: CM 2  
YIELD 48%

RX(1) RCT A 97-67-6, B 67-56-1  
RGT D 7719-09-7 SOCl2  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

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```
RX(7)      RCT  T 609846-34-6, U 585-79-5
           RGT  W 534-17-8 Cs2CO3
           PRO  V 609846-35-7
           CAT  161265-03-8 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-
           diyl)bis[1,1-diphenyl-, 3375-31-3 Pd(OAc)2
           SOL  108-88-3 PhMe
           CON  SUBSTAGE(1) room temperature
                SUBSTAGE(2) room temperature -> 95 deg C
                SUBSTAGE(3) 19 hours, 95 deg C

RX(44)     RCT  V 609846-35-7

           STAGE(1)
             RGT  BW 1310-65-2 LiOH
             SOL  7732-18-5 Water, 67-56-1 MeOH
             CON  room temperature

           STAGE(2)
             RGT  BX 7647-01-0 HCl
             SOL  7732-18-5 Water
             CON  room temperature

           STAGE(3)
             RCT  CL 172348-75-3
             RGT  CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
             1-[bis(dimethylamino)methylene]-, 3-oxide,
             hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
             SOL  68-12-2 DMF
             CON  100 minutes, room temperature

           PRO  CM 609846-74-4

RX(69)     RCT  CM 609846-74-4

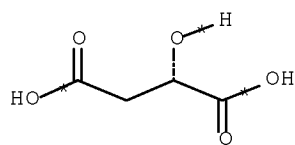
           STAGE(1)
             RGT  R 1333-74-0 H2
             CAT  7440-05-3 Pd
             SOL  7732-18-5 Water, 64-17-5 EtOH
             CON  1 hour, room temperature

           STAGE(2)
             RCT  DM 64-19-7
             SOL  7732-18-5 Water, 67-56-1 MeOH

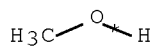
           PRO  DN 609847-00-9

RX(614) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(8),
           RX(31), RX(45)
RX(614)  2 A + 4 B + 2 E + 2 G + 3 Z + CL ==>
           CO
```

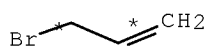
10/595943



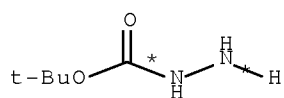
2 A



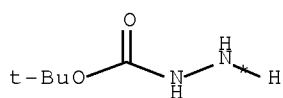
4 B



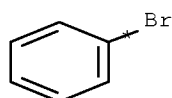
2 E



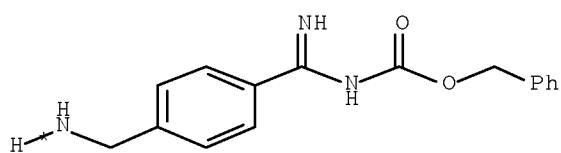
O



O



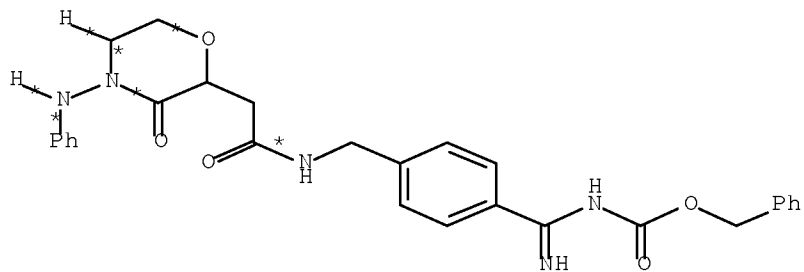
3 Z



CL

● 2 HCl

9  
STEPS  
→



CO

RX(1) RCT A 97-67-6, B 67-56-1

RGT D 7719-09-7 SOCl2

PRO C 617-55-0

CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6

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RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)

RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)

RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(8) RCT T 609846-34-6, Z 108-86-1  
RGT W 534-17-8 Cs2CO3  
PRO AA 609846-36-8, AB 609847-53-2  
CAT 161265-03-8 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-diyl)bis[1,1-diphenyl-, 3375-31-3 Pd(OAc)2  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 95 deg C  
SUBSTAGE(3) 19 hours, 95 deg C

RX(31) RCT AB 609847-53-2

STAGE(1)

RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water

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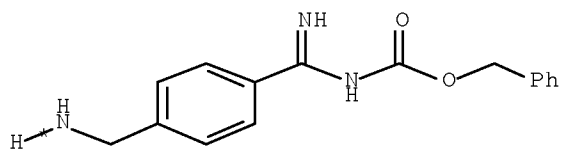
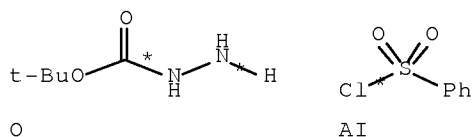
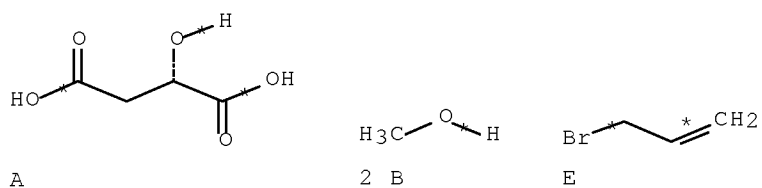
CON room temperature

PRO BY 609846-61-9

RX(45) RCT BY 609846-61-9, CL 172348-75-3  
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
 1-[bis(dimethylamino)methylene]-, 3-oxide,  
 hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
 PRO CO 609846-75-5  
 SOL 68-12-2 DMF  
 CON 100 minutes, room temperature

RX(615) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(12),  
 RX(35), RX(50)

RX(615) A + 2 B + E + O + AI + CL ==>  
 CT

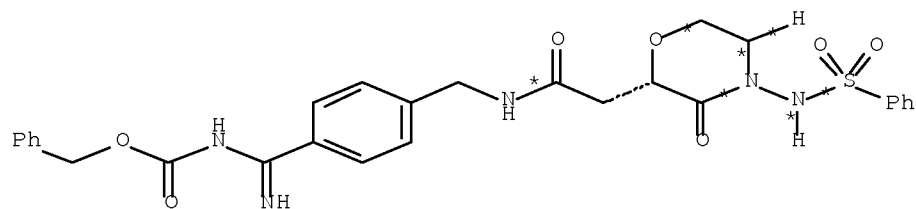


● 2 HCl

9  
 STEPS  
 →



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CT

RX(1) RCT A ~~97-67-6~~, B 67-56-1  
RGT D 7719-09-7 SOCl2  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K ~~7790-28-5~~ NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O ~~870-46-2~~  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C  
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

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RX(12) RCT T 609846-34-6, AI 98-09-9  
 PRO AK 609846-40-4  
 SOL 110-86-1 Pyridine  
 CON 20 hours, room temperature

RX(35) RCT AK 609846-40-4

STAGE(1)

RGT BW 1310-65-2 LiOH  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON room temperature

STAGE(2)

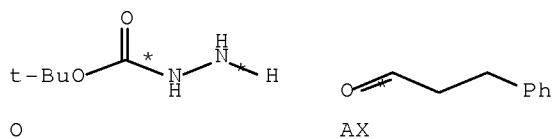
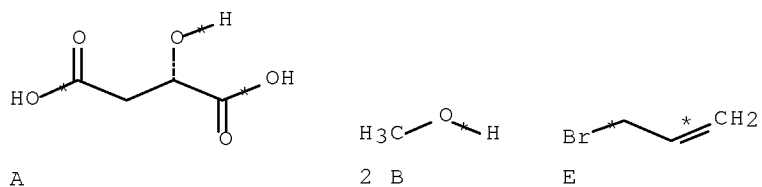
RGT BX 7647-01-0 HCl  
 SOL 7732-18-5 Water  
 CON room temperature

PRO CC 609846-65-3

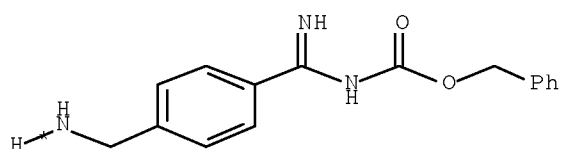
RX(50) RCT CC 609846-65-3, CL 172348-75-3  
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
 1-[bis(dimethylamino)methylene]-, 3-oxide,  
 hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
 PRO CT 609846-80-2  
 SOL 68-12-2 DMF  
 CON 100 minutes, room temperature

RX(616) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(21),  
 RX(42), RX(59)

RX(616) A + 2 B + E + O + AX + CL ==>  
 DC



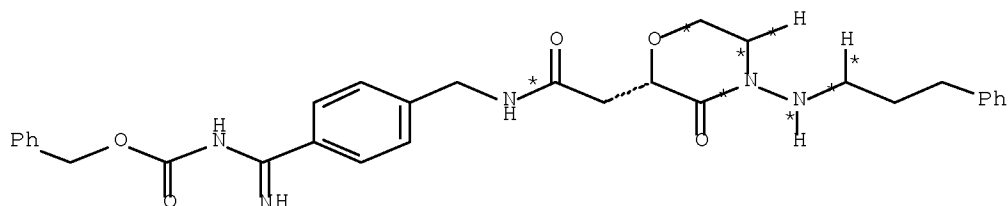
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CL

● 2 HCl

9  
STEPS  
→



DC

RX(1) RCT A 97-67-6, B 67-56-1  
RGT D 7719-09-7 SOCl2  
PRO C 617-55-0  
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6  
RGT G 20667-12-3 Ag2O  
PRO F 297749-53-2  
SOL 108-88-3 PhMe  
CON room temperature  
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)  
RGT J 7529-22-8 Me-morpholineoxide  
CAT 20816-12-0 OsO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

STAGE(2)  
RGT K 7790-28-5 NaIO4  
SOL 7732-18-5 Water, 109-99-9 THF  
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2  
PRO P 609846-32-4  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> 65 deg C

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SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4  
RGT R 1333-74-0 H2  
PRO Q 609846-33-5  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5  
PRO T 609846-34-6  
SOL 7732-18-5 Water  
CON 7 hours, 60 deg C  
NTE key intermediate

RX(21) RCT T 609846-34-6, AX 104-53-0

STAGE(1)  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) 5 hours, 70 deg C

STAGE(2)  
RGT R 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 109-99-9 THF  
CON 3 hours, room temperature

PRO BA 609846-50-6

RX(42) RCT BA 609846-50-6

STAGE(1)  
RGT BW 1310-65-2 LiOH  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

STAGE(2)  
RGT BX 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

PRO CJ 609846-72-2

RX(59) RCT CJ 609846-72-2, CL 172348-75-3  
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, 3-oxide,  
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2  
PRO DC ~~609846-89-1~~  
SOL 68-12-2 DMF  
CON 100 minutes, room temperature

L91 ANSWER 13 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 122:214089 CASREACT Full-text

TITLE: Novel synthesis of  
[(tetrazolylbiphenyl)methyl]tetraazacyclopentanaphth  
alenone

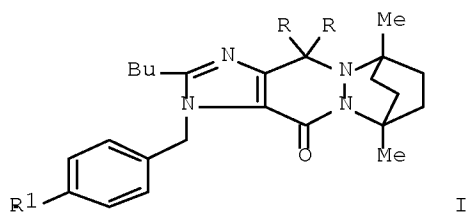
INVENTOR(S): Yamada, Hiroyoshi; Munesada, Kiyotaka; Koh, Keiko;  
Tsuzuki, Kazuo; Taniguchi, Mikio; Fujita, Yoshiji

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PATENT ASSIGNEE(S): Upjohn Co., USA  
 SOURCE: PCT Int. Appl., 18 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9500517	A1	19950105	WO 1994-US6028	19940602
W: AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, GE, HU, JP, KG, KP, KR, KZ, LK, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
JP 07010879	A	19950113	JP 1993-149132	19930621
AU 9470967	A	19950117	AU 1994-70967	19940602
EP 705266	A1	19960410	EP 1994-920047	19940602
EP 705266	B1	19970226		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 08512029	T	19961217	JP 1995-502833	19940602
JP 3391402	B2	20030331		
AT 149168	T	19970315	AT 1994-920047	19940602
ES 2099621	T3	19970516	ES 1994-920047	19940602
US 6005105	A	19991221	US 1995-557072	19951206
PRIORITY APPLN. INFO.:			JP 1993-149132	19930621
			WO 1994-US6028	19940602

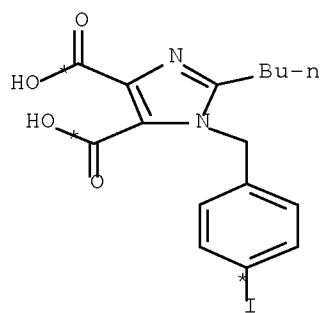
GI



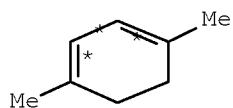
AB Halobenzyltetraazacyclopentanaphthalenedione I (RR = O, R1 = iodo)(preparation given) was condensed with 5-phenyl-1-triphenylmethyl-1H-tetrazole to give, after reduction and deprotection, I (R = H, R1 = 2-tetrazol-5-ylphenyl).

RX(17) OF 28 COMPOSED OF RX(1), RX(2), RX(3), RX(7)  
 RX(17) A + E + Z ==> N

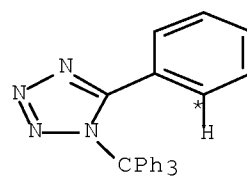
10/595943



A



E



Z

4  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(1) RCT A 161800-09-5

STAGE(1)

RGT C 302-01-2 N<sub>2</sub>H<sub>4</sub>

STAGE(2)

RGT D 7732-18-5 Water

PRO B 161800-10-8

RX(2) RCT B 161800-10-8, E 26120-52-5

STAGE(1)

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(2)

RGT G 546-67-8 Pb(OAc)<sub>4</sub>

STAGE(3)

SOL 108-88-3 PhMe

PRO F 161800-11-9

RX(3) RCT F 161800-11-9

STAGE(1)

RGT K 1576-35-8 Tosylhydrazide

SOL 68-12-2 DMF

STAGE(2)

SOL 141-78-6 AcOEt, 7732-18-5 Water

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PRO J 161800-12-0

RX(7) RCT Z 154750-11-5

STAGE(1)

RGT AA 109-72-8 BuLi

SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)

RGT AB 7646-85-7 ZnCl2

SOL 109-99-9 THF

STAGE(3)

RGT AC 676-58-4 MeMgCl

CAT 14264-16-5 NiCl2(PPh3)2

SOL 109-99-9 THF

STAGE(4)

RCT J 161800-12-0

SOL 109-99-9 THF

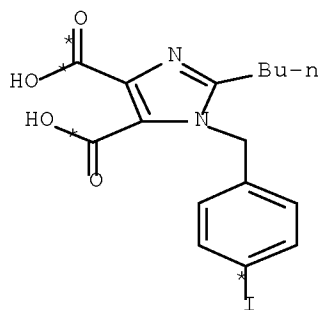
STAGE(5)

RGT AD 64-19-7 AcOH

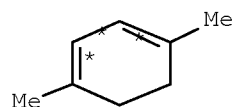
PRO N 161800-13-1

RX(23) OF 28 COMPOSED OF RX(1), RX(2), RX(3), RX(7), RX(4)

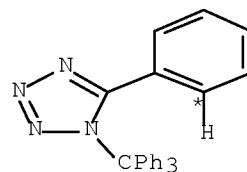
RX(23) A + E + Z ==> O



A



E



Z

5  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

10/595943

RX(1) RCT A 161800-09-5

STAGE(1)

RGT C 302-01-2 N2H4

STAGE(2)

RGT D 7732-18-5 Water

PRO B 161800-10-8

RX(2) RCT B 161800-10-8, E 26120-52-5

STAGE(1)

SOL 75-09-2 CH2Cl2

STAGE(2)

RGT G 546-67-8 Pb(OAc)4

STAGE(3)

SOL 108-88-3 PhMe

PRO F 161800-11-9

RX(3) RCT F 161800-11-9

STAGE(1)

RGT K 1576-35-8 Tosylhydrazide

SOL 68-12-2 DMF

STAGE(2)

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO J 161800-12-0

RX(7) RCT Z 154750-11-5

STAGE(1)

RGT AA 109-72-8 BuLi

SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)

RGT AB 7646-85-7 ZnCl2

SOL 109-99-9 THF

STAGE(3)

RGT AC 676-58-4 MeMgCl

CAT 14264-16-5 NiCl2(PPh3)2

SOL 109-99-9 THF

STAGE(4)

RCT J 161800-12-0

SOL 109-99-9 THF

STAGE(5)

RGT AD 64-19-7 AcOH

PRO N 161800-13-1

RX(4) RCT N 161800-13-1



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STAGE(1)

SOL 109-99-9 THF

STAGE(2)

RGT P 1191-15-7  $\text{AlH}(\text{Bu-i})_2$

SOL 108-88-3 PhMe

STAGE(3)

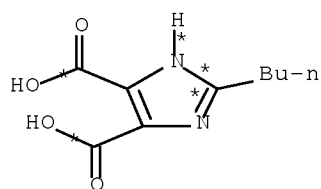
RGT Q 7647-14-5 NaCl

SOL 7732-18-5 Water

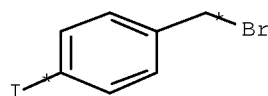
PRO O 161800-14-2

RX(24) OF 28 COMPOSED OF RX(6), RX(1), RX(2), RX(3), RX(7)

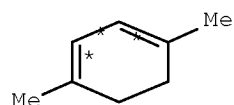
RX(24) V + W + E + Z ==> N



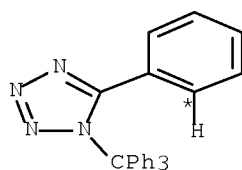
V



W

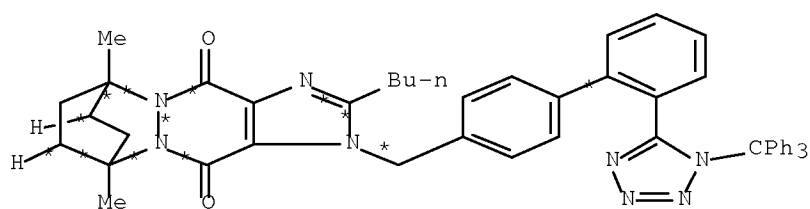


E



Z

5  
STEPS  
→



N  
YIELD 77%

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RX(6) RCT V ~~71998-99-7~~, W 16004-15-2

STAGE(1)

RGT X ~~7646-69-7~~ NaH

SOL ~~68-12-2~~ DMF

STAGE(2)

RGT Y ~~67-56-1~~ MeOH

PRO A 161800-09-5

RX(1) RCT A 161800-09-5

STAGE(1)

RGT C ~~302-01-2~~ N2H4

STAGE(2)

RGT D ~~7732-18-5~~ Water

PRO B 161800-10-8

RX(2) RCT B 161800-10-8, E 26120-52-5

STAGE(1)

SOL ~~75-09-2~~ CH2Cl2

STAGE(2)

RGT G ~~546-67-8~~ Pb(OAc)4

STAGE(3)

SOL ~~108-88-3~~ PhMe

PRO F 161800-11-9

RX(3) RCT F 161800-11-9

STAGE(1)

RGT K ~~1576-35-8~~ Tosylhydrazide

SOL ~~68-12-2~~ DMF

STAGE(2)

SOL ~~141-78-6~~ AcOEt, ~~7732-18-5~~ Water

PRO J 161800-12-0

RX(7) RCT Z 154750-11-5

STAGE(1)

RGT AA ~~109-72-8~~ BuLi

SOL ~~109-99-9~~ THF, ~~110-54-3~~ Hexane

STAGE(2)

RGT AB ~~7646-85-7~~ ZnCl2

SOL ~~109-99-9~~ THF

STAGE(3)

RGT AC ~~676-58-4~~ MeMgCl

CAT ~~14264-16-5~~ NiCl2(PPh3)2

SOL ~~109-99-9~~ THF

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STAGE(4)

RCT J 161800-12-0

SOL 109-99-9 THF

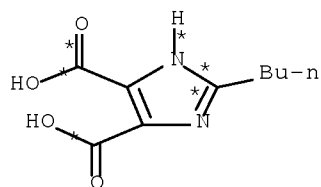
STAGE(5)

RGT AD 64-19-7 AcOH

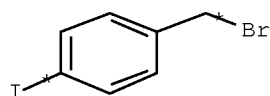
PRO N 161800-13-1

RX(25) OF 28 COMPOSED OF RX(6), RX(1), RX(2), RX(3), RX(7), RX(4)

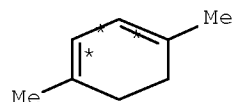
RX(25) V + W + E + Z ==> O



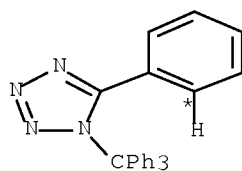
V



W

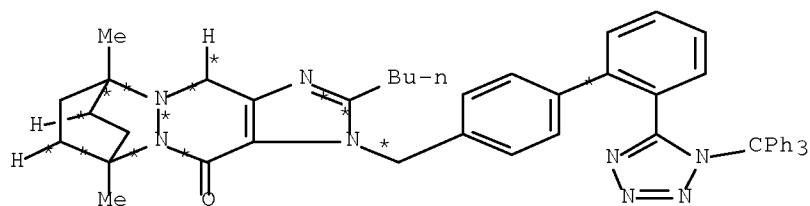


E



Z

6  
STEPS  
→



O  
YIELD 97%

RX(6) RCT V 71998-99-7, W 16004-15-2

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```

      STAGE(1)
        RGT  X 7646-69-7 NaH
        SOL  68-12-2 DMF

      STAGE(2)
        RGT  Y 67-56-1 MeOH

PRO   A 161800-09-5

RX(1)  RCT  A 161800-09-5

      STAGE(1)
        RGT  C 302-01-2 N2H4

      STAGE(2)
        RGT  D 7732-18-5 Water

PRO   B 161800-10-8

RX(2)  RCT  B 161800-10-8, E 26120-52-5

      STAGE(1)
        SOL  75-09-2 CH2Cl2

      STAGE(2)
        RGT  G 546-67-8 Pb(OAc)4

      STAGE(3)
        SOL  108-88-3 PhMe

PRO   F 161800-11-9

RX(3)  RCT  F 161800-11-9

      STAGE(1)
        RGT  K 1576-35-8 Tosylhydrazide
        SOL  68-12-2 DMF

      STAGE(2)
        SOL  141-78-6 AcOEt, 7732-18-5 Water

PRO   J 161800-12-0

RX(7)  RCT  Z 154750-11-5

      STAGE(1)
        RGT  AA 109-72-8 BuLi
        SOL  109-99-9 THF, 110-54-3 Hexane

      STAGE(2)
        RGT  AB 7646-85-7 ZnCl2
        SOL  109-99-9 THF

      STAGE(3)
        RGT  AC 676-58-4 MeMgCl
        CAT  14264-16-5 NiCl2(PPh3)2
        SOL  109-99-9 THF

      STAGE(4)
        RCT  J 161800-12-0
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SOL 109-99-9 THF

STAGE(5)

RGT AD 64-19-7 AcOH

PRO N 161800-13-1

RX(4) RCT N 161800-13-1

STAGE(1)

SOL 109-99-9 THF

STAGE(2)

RGT P 1191-15-7 AlH(Bu-i)2

SOL 108-88-3 PhMe

STAGE(3)

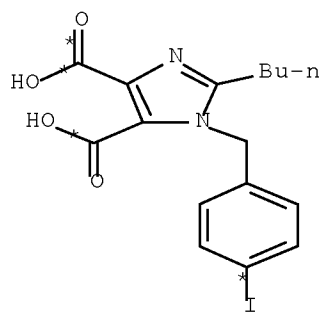
RGT Q 7647-14-5 NaCl

SOL 7732-18-5 Water

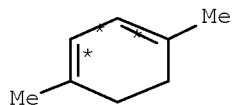
PRO O 161800-14-2

RX(27) OF 28 COMPOSED OF RX(1), RX(2), RX(3), RX(7), RX(4), RX(5)

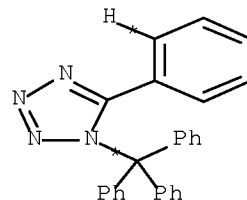
RX(27) A + E + Z ==> S



A



E



Z

6  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(1) RCT A 161800-09-5

STAGE(1)

RGT C 302-01-2 N2H4

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```
      STAGE(2)
      RGT  D 7732-18-5 Water

PRO   B 161800-10-8

RX(2)  RCT  B 161800-10-8, E 26120-52-5

      STAGE(1)
      SOL  75-09-2 CH2Cl2

      STAGE(2)
      RGT  G 546-67-8 Pb(OAc)4

      STAGE(3)
      SOL  108-88-3 PhMe

PRO   F 161800-11-9

RX(3)  RCT  F 161800-11-9

      STAGE(1)
      RGT  K 1576-35-8 Tosylhydrazide
      SOL  68-12-2 DMF

      STAGE(2)
      SOL  141-78-6 AcOEt, 7732-18-5 Water

PRO   J 161800-12-0

RX(7)  RCT  Z 154750-11-5

      STAGE(1)
      RGT  AA 109-72-8 BuLi
      SOL  109-99-9 THF, 110-54-3 Hexane

      STAGE(2)
      RGT  AB 7646-85-7 ZnCl2
      SOL  109-99-9 THF

      STAGE(3)
      RGT  AC 676-58-4 MeMgCl
      CAT  14264-16-5 NiCl2(PPh3)2
      SOL  109-99-9 THF

      STAGE(4)
      RCT  J 161800-12-0
      SOL  109-99-9 THF

      STAGE(5)
      RGT  AD 64-19-7 AcOH

PRO   N 161800-13-1

RX(4)  RCT  N 161800-13-1

      STAGE(1)
      SOL  109-99-9 THF

      STAGE(2)
      RGT  P 1191-15-7 AlH(Bu-i)2
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SOL 108-88-3 PhMe

STAGE(3)

RGT Q 7647-14-5 NaCl

SOL 7732-18-5 Water

PRO O 161800-14-2

RX(5) RCT O 161800-14-2

STAGE(1)

RGT T 7647-01-0 HCl

SOL 67-64-1 Me2CO

STAGE(2)

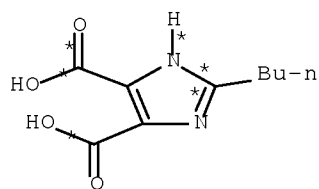
RGT Q 7647-14-5 NaCl

SOL 7732-18-5 Water

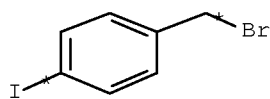
PRO S 152134-03-7

RX(28) OF 28 COMPOSED OF RX(6), RX(1), RX(2), RX(3), RX(7), RX(4), RX(5)

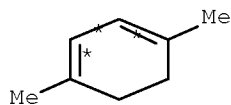
RX(28) V + W + E + Z ==> S



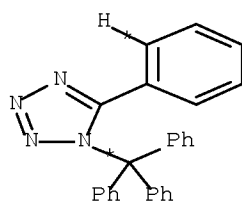
V



W



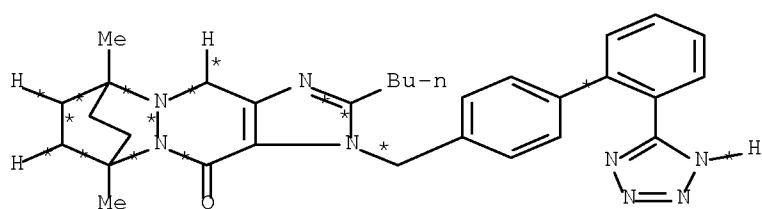
E



Z

7  
STEPS  
→

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S  
YIELD 91%

RX(6) RCT V 71998-99-7, W 16004-15-2

STAGE(1)

RGT X 7646-69-7 NaH

SOL 68-12-2 DMF

STAGE(2)

RGT Y 67-56-1 MeOH

PRO A 161800-09-5

RX(1) RCT A 161800-09-5

STAGE(1)

RGT C 302-01-2 N2H4

STAGE(2)

RGT D 7732-18-5 Water

PRO B 161800-10-8

RX(2) RCT B 161800-10-8, E 26120-52-5

STAGE(1)

SOL 75-09-2 CH2Cl2

STAGE(2)

RGT G 546-67-8 Pb(OAc)4

STAGE(3)

SOL 108-88-3 PhMe

PRO F 161800-11-9

RX(3) RCT F 161800-11-9

STAGE(1)

RGT K 1576-35-8 Tosylhydrazide

SOL 68-12-2 DMF

STAGE(2)

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO J 161800-12-0



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RX(7) RCT Z 154750-11-5

STAGE(1)

RGT AA 109-72-8 BuLi

SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)

RGT AB ~~7646-85-7~~ ZnCl<sub>2</sub>

SOL 109-99-9 THF

STAGE(3)

RGT AC 676-58-4 MeMgCl

CAT ~~14264-16-5~~ NiCl<sub>2</sub>(PPh<sub>3</sub>)<sub>2</sub>

SOL 109-99-9 THF

STAGE(4)

RCT J 161800-12-0

SOL 109-99-9 THF

STAGE(5)

RGT AD 64-19-7 AcOH

PRO N 161800-13-1

RX(4) RCT N 161800-13-1

STAGE(1)

SOL 109-99-9 THF

STAGE(2)

RGT P 1191-15-7 AlH(Bu-i)<sub>2</sub>

SOL 108-88-3 PhMe

STAGE(3)

RGT Q ~~7647-14-5~~ NaCl

SOL 7732-18-5 Water

PRO O 161800-14-2

RX(5) RCT O 161800-14-2

STAGE(1)

RGT T 7647-01-0 HCl

SOL 67-64-1 Me<sub>2</sub>CO

STAGE(2)

RGT Q ~~7647-14-5~~ NaCl

SOL 7732-18-5 Water

PRO S ~~152134-03-7~~

L91 ANSWER 14 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 122:106074 CASREACT Full-text

TITLE: Ferrocenes and ferrocenophanes with dipolar structure elements

AUTHOR(S): Pagel, Karsten; Werner, Andreas; Friedrichsen, Willy

CORPORATE SOURCE: Institut fuer Organische Chemie der Universitaet Kiel, Olshausenstrasse 40-60, Kiel, D-24018, Germany

SOURCE: Journal of Organometallic Chemistry (1994), 481(1),

10/595943

109-23

CODEN: JORCAI; ISSN: 0022-328X

PUBLISHER:

Elsevier

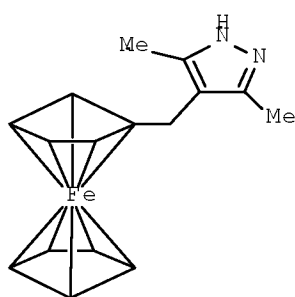
DOCUMENT TYPE:

Journal

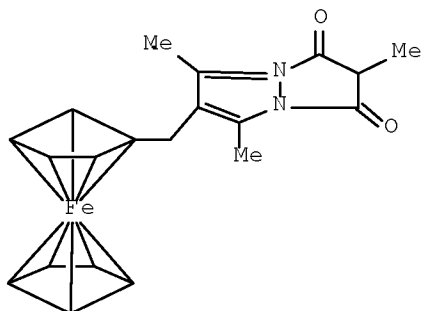
LANGUAGE:

German

GI



I

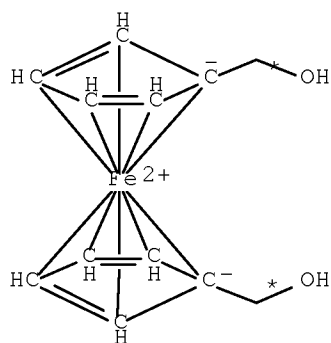


II

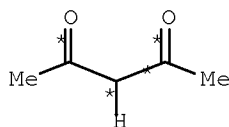
AB The synthesis of ferrocenyl substituted pyrazoles, e.g. I, and the subsequent reaction of these compds. with reactive malonic acid derivs. yielding dipolaric pyrazolo[1,2-a]pyrazol-4-ium-3-olates, e.g. II, is described.

RX(87) OF 260 COMPOSED OF RX(4), RX(5), RX(21)

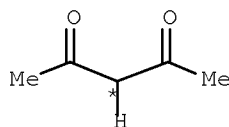
RX(87) L + 2 M + 2 AQ ==> AQ



L

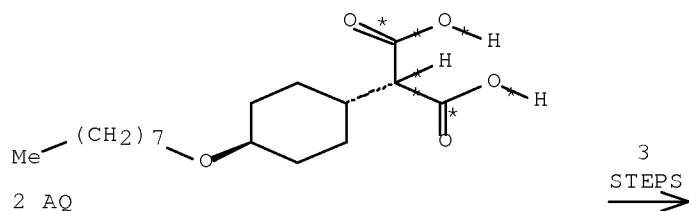


M



M

10/595943



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(4) RCT L 1291-48-1, M 123-54-6  
RGT O 16872-11-0 HBF<sub>4</sub>  
PRO N 160791-68-4  
SOL 7732-18-5 Water

RX(5) RCT N 160791-68-4  
RGT F 302-01-2 N<sub>2</sub>H<sub>4</sub>  
PRO Q 160791-69-5  
SOL 64-17-5 EtOH

RX(21) RCT AQ 123854-20-6

STAGE(1)  
RGT AS 7719-09-7 SOCl<sub>2</sub>

STAGE(2)  
SOL 109-99-9 THF

STAGE(3)  
RCT Q 160791-69-5  
SOL 109-99-9 THF

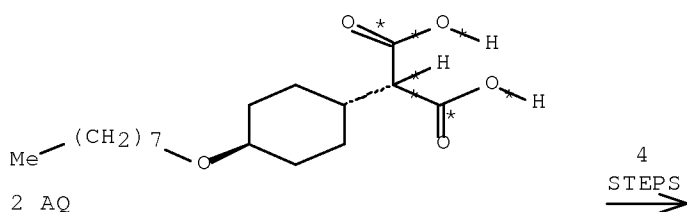
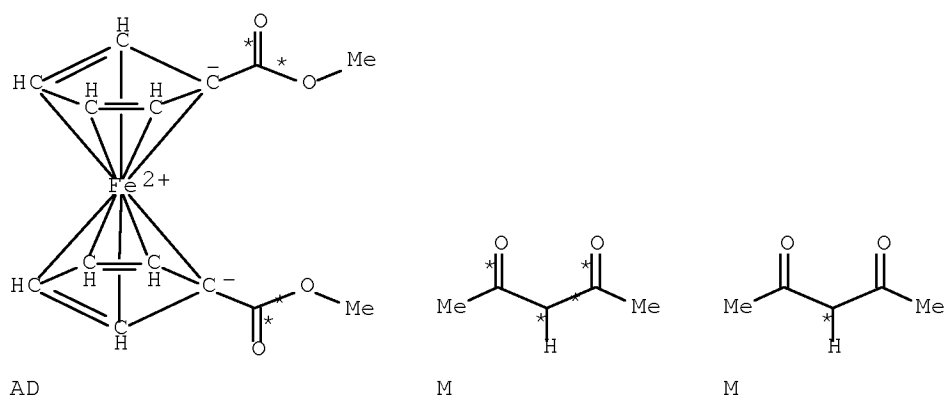
STAGE(4)  
RGT J 121-44-8 Et<sub>3</sub>N  
SOL 109-99-9 THF

PRO AU 160824-73-7

RX(90) OF 260 COMPOSED OF RX(9), RX(4), RX(5), RX(21)

RX(90) AD + 2 M + 2 AQ ==> AU

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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(9) RCT AD 1273-95-6  
RGT AB 16853-85-3 LiAlH4  
PRO L 1291-48-1  
SOL 109-99-9 THF

RX(4) RCT L 1291-48-1, M 123-54-6  
RGT O 16872-11-0 HBF4  
PRO N 160791-68-4  
SOL 7732-18-5 Water

RX(5) RCT N 160791-68-4  
RGT F 302-01-2 N2H4  
PRO Q 160791-69-5  
SOL 64-17-5 EtOH

RX(21) RCT AQ 123854-20-6

STAGE(1)  
RGT AS 7719-09-7 SOCl2

STAGE(2)  
SOL 109-99-9 THF

STAGE(3)  
RCT Q 160791-69-5

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SOL 109-99-9 THF

STAGE(4)

RGT J 121-44-8 Et3N

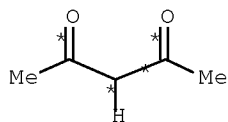
SOL 109-99-9 THF

PRO AU 160824-73-7

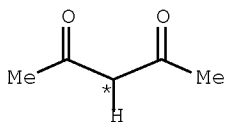
RX(101) OF 260 COMPOSED OF RX(11), RX(13), RX(22)

RX(101) AE + 2 M + 2 AV ==> AW

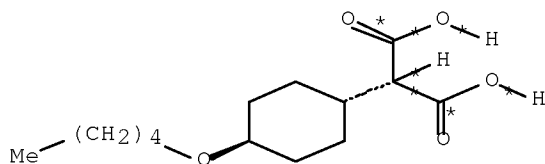
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*



M



M



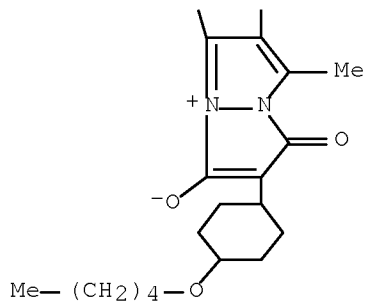
2 AV

3  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

PAGE 3-A



AW  
YIELD 43%

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RX(11) RCT AE 108693-71-6, M 123-54-6  
RGT O 16872-11-0 HBF4  
PRO AF 160791-70-8  
SOL 75-09-2 CH2Cl2  
NTE (16% CRYSTALS, 46% OIL)

RX(13) RCT AF 160791-70-8  
RGT F 302-01-2 N2H4  
PRO AH 160791-72-0  
SOL 64-17-5 EtOH

RX(22) RCT AV 160811-27-8

STAGE(1)  
RGT AS 7719-09-7 SOCl2

STAGE(2)  
SOL 109-99-9 THF

STAGE(3)  
RCT AH 160791-72-0  
SOL 109-99-9 THF

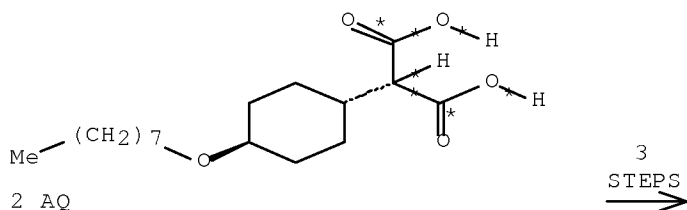
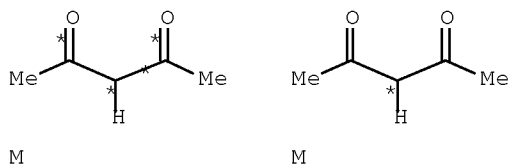
STAGE(4)  
RGT J 121-44-8 Et3N  
SOL 109-99-9 THF

PRO AW 160791-75-3

RX(102) OF 260 COMPOSED OF RX(11), RX(13), RX(24)

RX(102) AE + 2 M + 2 AQ ==> AY

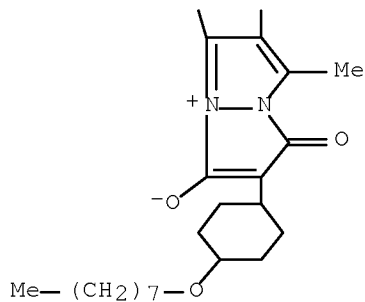
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

PAGE 3-A



AY  
YIELD 59%

RX(11) RCT AE 108693-71-6, M 123-54-6  
RGT O 16872-11-0 HBF4  
PRO AF 160791-70-8  
SOL 75-09-2 CH2Cl2  
NTE (16% CRYSTALS, 46% OIL)

RX(13) RCT AF 160791-70-8  
RGT F 302-01-2 N2H4  
PRO AH 160791-72-0  
SOL 64-17-5 EtOH

RX(24) RCT AQ 123854-20-6

STAGE(1)

RGT AS 7719-09-7 SOCl2

STAGE(2)

SOL 109-99-9 THF

STAGE(3)

RCT AH 160791-72-0

SOL 109-99-9 THF

STAGE(4)

RGT J 121-44-8 Et3N

SOL 109-99-9 THF

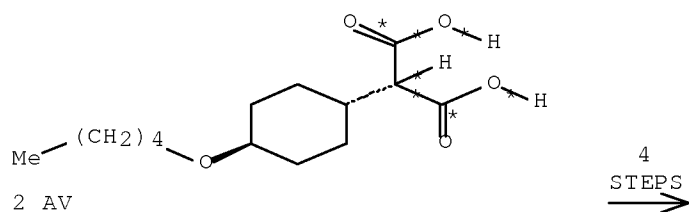
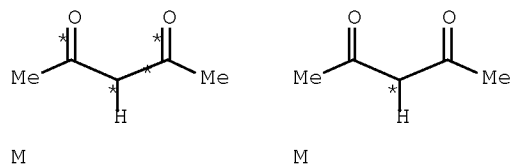
PRO AY 160791-77-5

RX(103) OF 260 COMPOSED OF RX(10), RX(11), RX(13), RX(22)

RX(103) W + 2 M + 2 AV ==> AW

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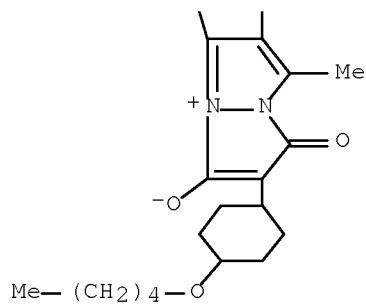
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

PAGE 3-A



AW  
YIELD 43%

RX(10) RCT W 82522-10-9  
RGT AB 16853-85-3 LiAlH<sub>4</sub>  
PRO AE 108693-71-6  
SOL 109-99-9 THF

RX(11) RCT AE 108693-71-6, M 123-54-6  
RGT O 16872-11-0 HBF<sub>4</sub>  
PRO AF 160791-70-8  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>



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NTE (16% CRYSTALS, 46% OIL)

RX(13) RCT AF 160791-70-8  
RGT F 302-01-2 N2H4  
PRO AH 160791-72-0  
SOL 64-17-5 EtOH

RX(22) RCT AV 160811-27-8

STAGE(1)  
RGT AS 7719-09-7 SOC12

STAGE(2)  
SOL 109-99-9 THF

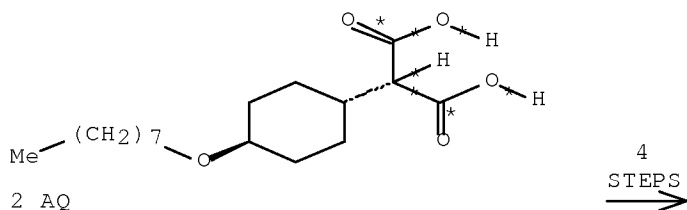
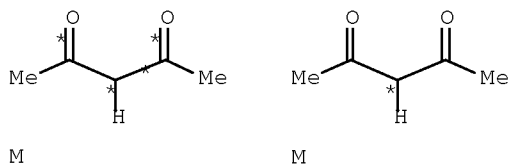
STAGE(3)  
RCT AH 160791-72-0  
SOL 109-99-9 THF

STAGE(4)  
RGT J 121-44-8 Et3N  
SOL 109-99-9 THF

PRO AW 160791-75-3

RX(104) OF 260 COMPOSED OF RX(10), RX(11), RX(13), RX(24)  
RX(104) W + 2 M + 2 AQ ==> AY

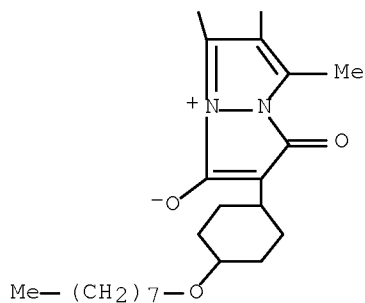
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*



4  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*



AY  
YIELD 59%

RX(10) RCT W 82522-10-9  
RGT AB 16853-85-3 LiAlH<sub>4</sub>  
PRO AE 108693-71-6  
SOL 109-99-9 THF

RX(11) RCT AE 108693-71-6, M 123-54-6  
RGT O 16872-11-0 HBF<sub>4</sub>  
PRO AF 160791-70-8  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
NTE (16% CRYSTALS, 46% OIL)

RX(13) RCT AF 160791-70-8  
RGT F 302-01-2 N<sub>2</sub>H<sub>4</sub>  
PRO AH 160791-72-0  
SOL 64-17-5 EtOH

RX(24) RCT AQ 123854-20-6

STAGE(1)  
RGT AS 7719-09-7 SOCl<sub>2</sub>

STAGE(2)  
SOL 109-99-9 THF

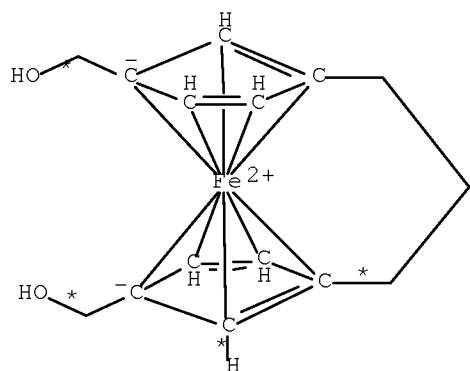
STAGE(3)  
RCT AH 160791-72-0  
SOL 109-99-9 THF

STAGE(4)  
RGT J 121-44-8 Et<sub>3</sub>N  
SOL 109-99-9 THF

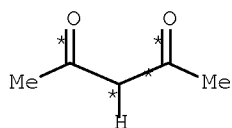
PRO AY 160791-77-5

RX(105) OF 260 COMPOSED OF RX(12), RX(14), RX(23)  
RX(105) AA + 2 M + 2 AV ==> AX

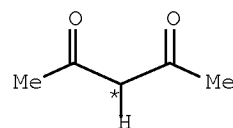
10/595943



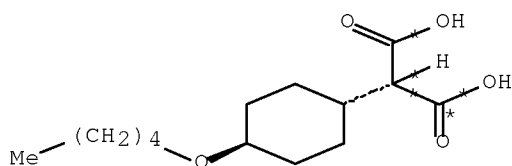
AA



M



M

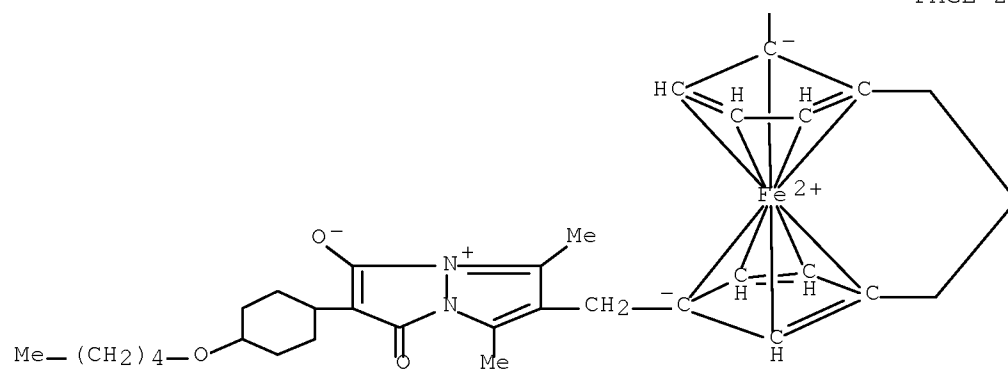


2 AV

3  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

PAGE 2-A



AX  
YIELD 38%

RX(12) RCT AA 108693-72-7, M 123-54-6  
RGT O 16872-11-0 HBF4  
PRO AG 160791-71-9

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SOL 75-09-2 CH2Cl2

RX(14) RCT AG 160791-71-9  
RGT F 302-01-2 N2H4  
PRO AI 160824-68-0  
SOL 64-17-5 EtOH

RX(23) RCT AV 160811-27-8

STAGE(1)  
RGT AS 7719-09-7 SOC12

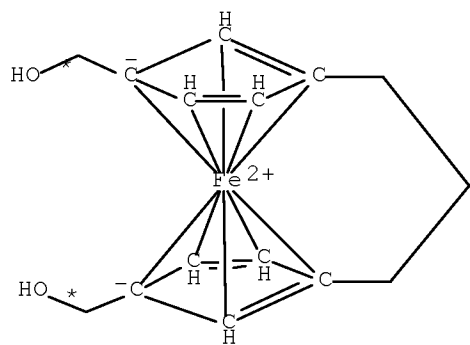
STAGE(2)  
SOL 109-99-9 THF

STAGE(3)  
RCT AI 160824-68-0  
SOL 109-99-9 THF

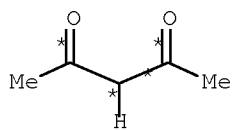
STAGE(4)  
RGT J 121-44-8 Et3N  
SOL 109-99-9 THF

PRO AX 160791-76-4

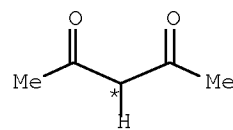
RX(106) OF 260 COMPOSED OF RX(12), RX(14), RX(25)  
RX(106) AA + 2 M + 2 AQ ==> AZ



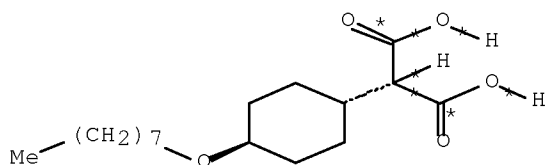
AA



M



M



2 AQ

3  
STEPS  
→

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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(12) RCT AA 108693-72-7, M 123-54-6  
RGT O 16872-11-0 HBF<sub>4</sub>  
PRO AG 160791-71-9  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

RX(14) RCT AG 160791-71-9  
RGT F 302-01-2 N<sub>2</sub>H<sub>4</sub>  
PRO AI 160824-68-0  
SOL 64-17-5 EtOH

RX(25) RCT AQ 123854-20-6

STAGE(1)  
RGT AS 7719-09-7 SOCl<sub>2</sub>

STAGE(2)  
SOL 109-99-9 THF

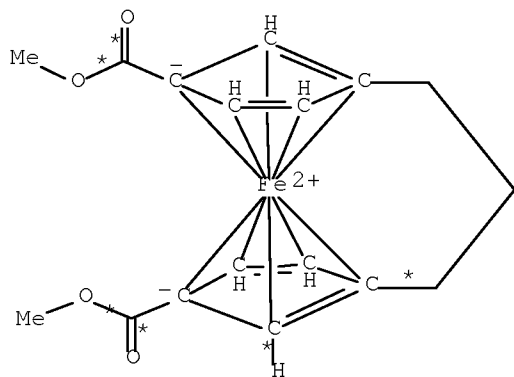
STAGE(3)  
RCT AI 160824-68-0  
SOL 109-99-9 THF

STAGE(4)  
RGT J 121-44-8 Et<sub>3</sub>N  
SOL 109-99-9 THF

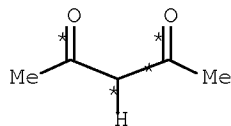
PRO AZ 160791-78-6

RX(107) OF 260 COMPOSED OF RX(8), RX(12), RX(14), RX(23)

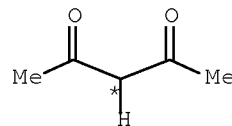
RX(107) X + 2 M + 2 AV ==> AX



X

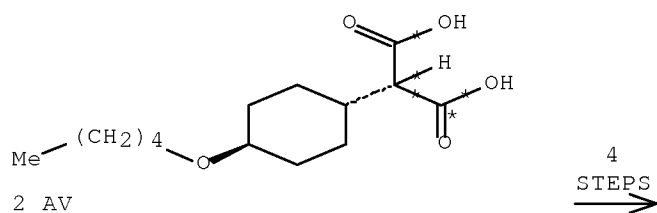


M



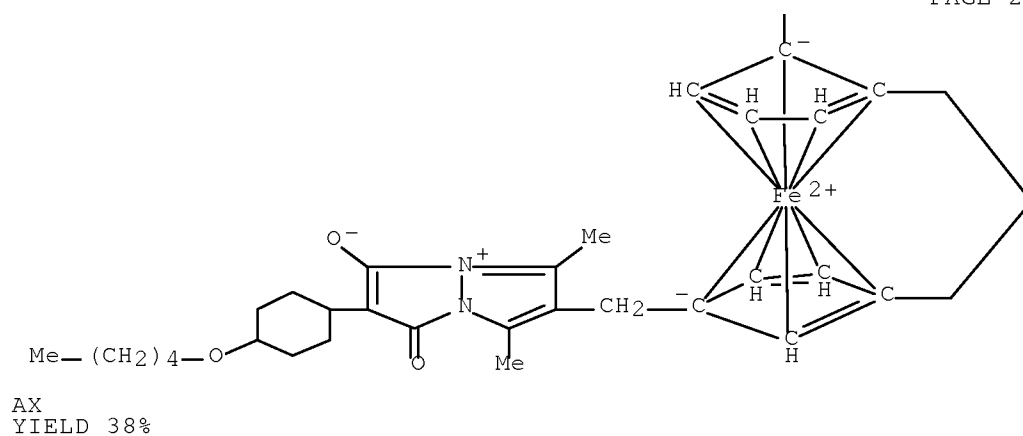
M

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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

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RX(8) RCT X 82544-17-0  
RGT AB 16853-85-3 LiAlH<sub>4</sub>  
PRO AA 108693-72-7  
SOL 109-99-9 THF

RX(12) RCT AA 108693-72-7, M 123-54-6  
RGT O 16872-11-0 HBF<sub>4</sub>  
PRO AG 160791-71-9  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

RX(14) RCT AG 160791-71-9  
RGT F 302-01-2 N<sub>2</sub>H<sub>4</sub>  
PRO AI 160824-68-0  
SOL 64-17-5 EtOH

RX(23) RCT AV 160811-27-8

STAGE(1)  
RGT AS 7719-09-7 SOCl<sub>2</sub>

STAGE(2)  
SOL 109-99-9 THF

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STAGE(3)

RCT AI 160824-68-0

SOL 109-99-9 THF

STAGE(4)

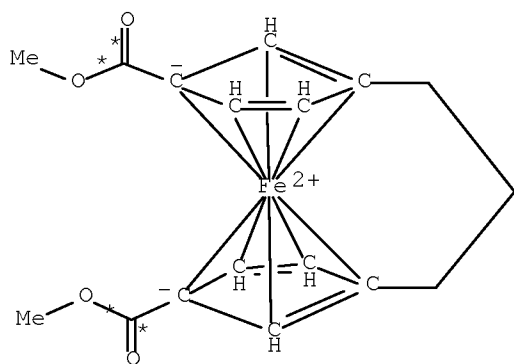
RGT J 121-44-8 Et3N

SOL 109-99-9 THF

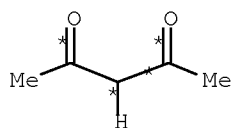
PRO AX 160791-76-4

RX(108) OF 260 COMPOSED OF RX(8), RX(12), RX(14), RX(25)

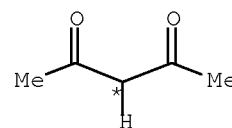
RX(108) X + 2 M + 2 AQ ==> AZ



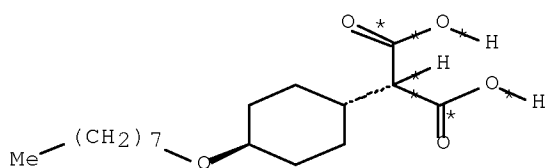
X



M



M



2 AQ

4  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(8)

RCT X 82544-17-0

RGT AB 16853-85-3 LiAlH4

PRO AA 108693-72-7

SOL 109-99-9 THF

RX(12)

RCT AA 108693-72-7, M 123-54-6

RGT O 16872-11-0 HBF4

PRO AG 160791-71-9

SOL 75-09-2 CH2Cl2

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RX(14) RCT AG 160791-71-9  
 RGT F 302-01-2 N2H4  
 PRO AI 160824-68-0  
 SOL 64-17-5 EtOH

RX(25) RCT AQ 123854-20-6

STAGE(1)  
 RGT AS 7719-09-7 SOC12

STAGE(2)  
 SOL 109-99-9 THF

STAGE(3)  
 RCT AI 160824-68-0  
 SOL 109-99-9 THF

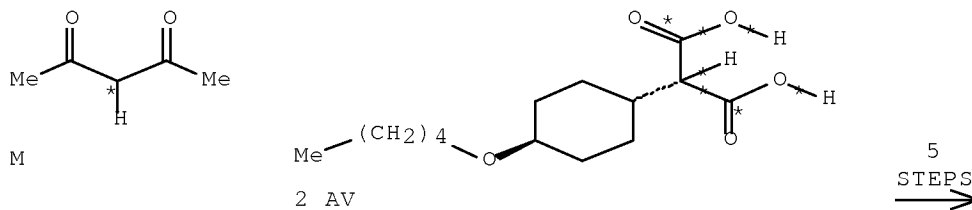
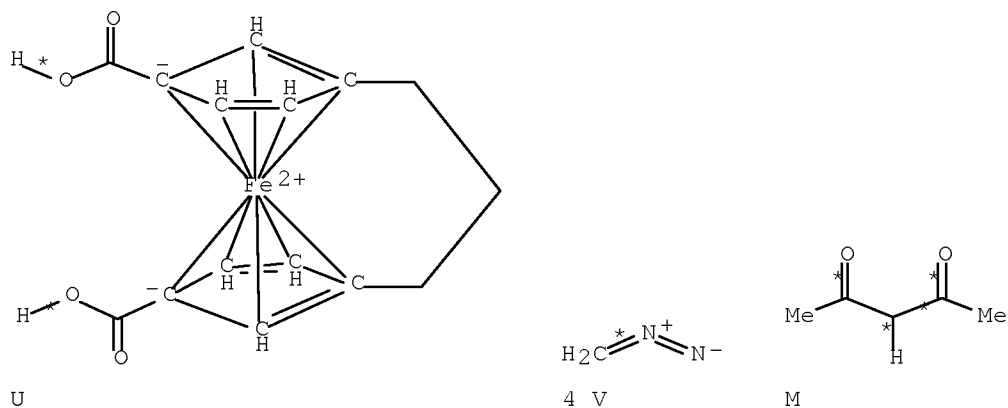
STAGE(4)  
 RGT J 121-44-8 Et3N  
 SOL 109-99-9 THF

PRO AZ 160791-78-6

RX(160) OF 260 COMPOSED OF RX(7), RX(10), RX(11), RX(13), RX(22)

RX(160) T + U + 4 V + 2 M + 2 AV ==> AW

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

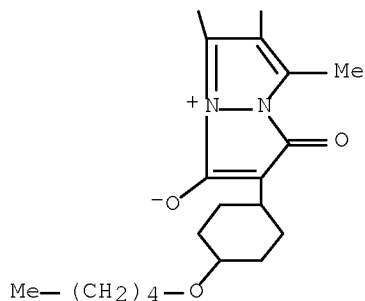




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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

PAGE 3-A



AW  
YIELD 43%

RX(7) RCT T 155565-57-4, U 155565-58-5, V 334-88-3  
PRO W 82522-10-9, X 82544-17-0  
SOL 67-56-1 MeOH, 60-29-7 Et2O

RX(10) RCT W 82522-10-9  
RGT AB 16853-85-3 LiAlH4  
PRO AE 108693-71-6  
SOL 109-99-9 THF

RX(11) RCT AE 108693-71-6, M 123-54-6  
RGT O ~~16872-11-0~~ HBF4  
PRO AF 160791-70-8  
SOL 75-09-2 CH2Cl2  
NTE (16% CRYSTALS, 46% OIL)

RX(13) RCT AF 160791-70-8  
RGT F ~~302-01-2~~ N2H4  
PRO AH 160791-72-0  
SOL 64-17-5 EtOH

RX(22) RCT AV ~~160811-27-8~~

STAGE(1)  
RGT AS 7719-09-7 SOCl2

STAGE(2)  
SOL 109-99-9 THF

STAGE(3)  
RCT AH 160791-72-0  
SOL 109-99-9 THF

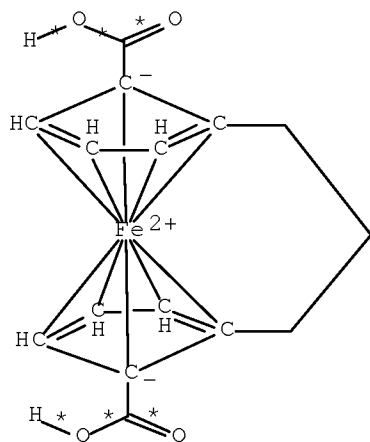
STAGE(4)  
RGT J 121-44-8 Et3N

10/595943

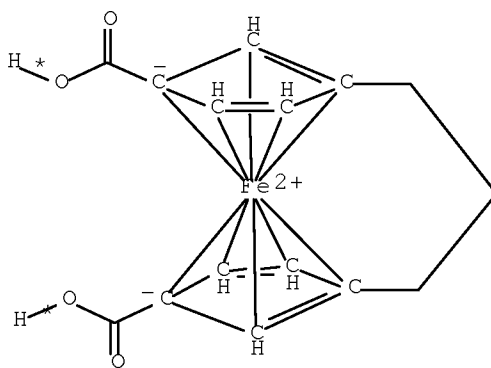
SOL 109-99-9 THF

PRO AW 160791-75-3

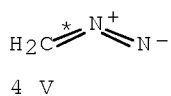
RX(161) OF 260 COMPOSED OF RX(7), RX(10), RX(11), RX(13), RX(24)  
 RX(161) T + U + 4 V + 2 M + 2 AQ ==> AY



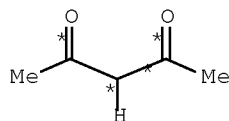
T



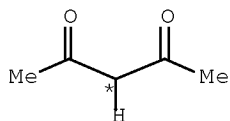
U



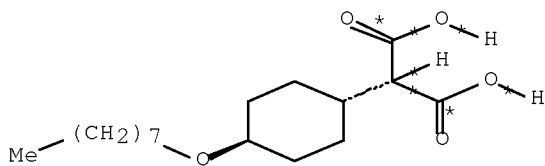
4 V



M



M

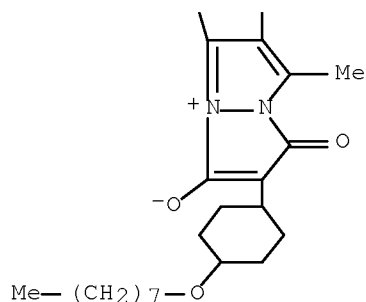


2 AQ

5  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*



AY  
YIELD 59%

RX(7) RCT T 155565-57-4, U 155565-58-5, V 334-88-3  
PRO W 82522-10-9, X 82544-17-0  
SOL 67-56-1 MeOH, 60-29-7 Et2O

RX(10) RCT W 82522-10-9  
RGT AB 16853-85-3 LiAlH<sub>4</sub>  
PRO AE 108693-71-6  
SOL 109-99-9 THF

RX(11) RCT AE 108693-71-6, M 123-54-6  
RGT O 16872-11-0 HBF<sub>4</sub>  
PRO AF 160791-70-8  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
NTE (16% CRYSTALS, 46% OIL)

RX(13) RCT AF 160791-70-8  
RGT F 302-01-2 N<sub>2</sub>H<sub>4</sub>  
PRO AH 160791-72-0  
SOL 64-17-5 EtOH

RX(24) RCT AQ 123854-20-6

STAGE(1)  
RGT AS 7719-09-7 SOCl<sub>2</sub>

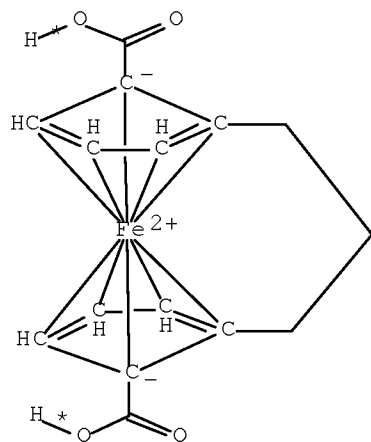
STAGE(2)  
SOL 109-99-9 THF

STAGE(3)  
RCT AH 160791-72-0  
SOL 109-99-9 THF

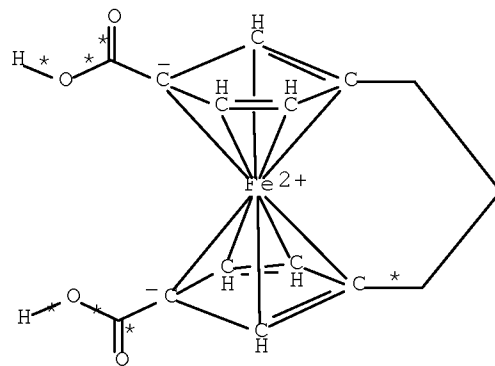
STAGE(4)  
RGT J 121-44-8 Et<sub>3</sub>N  
SOL 109-99-9 THF

PRO AY 160791-77-5

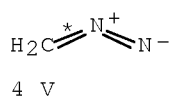
RX(162) OF 260 COMPOSED OF RX(7), RX(8), RX(12), RX(14), RX(23)  
RX(162) T + U + 4 V + 2 M + 2 AV ==> AX



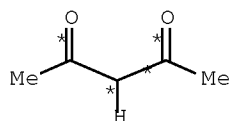
T



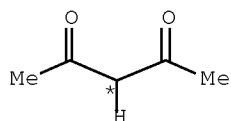
U



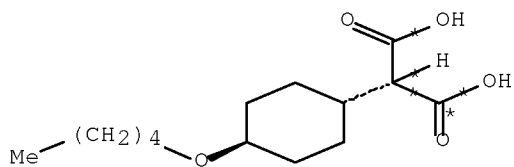
4 V



M



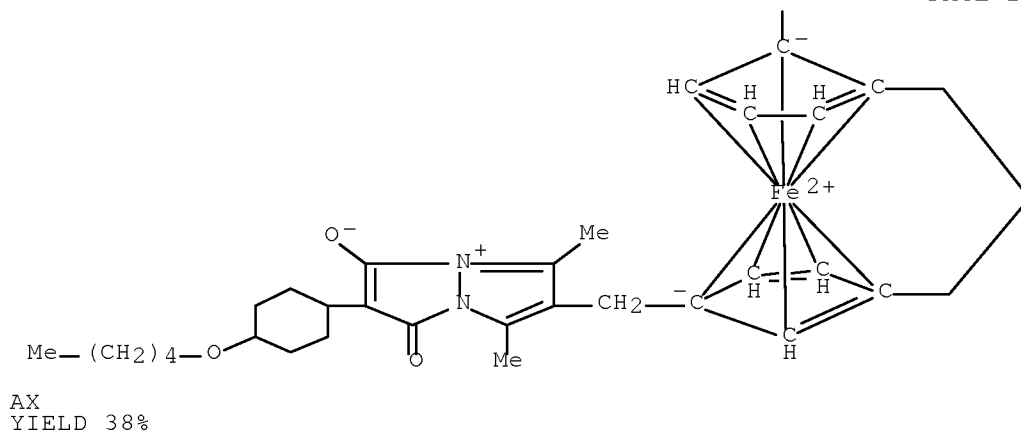
M



2 AV

5  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*



RX(7) RCT T 155565-57-4, U 155565-58-5, V 334-88-3  
PRO W 82522-10-9, X 82544-17-0  
SOL 67-56-1 MeOH, 60-29-7 Et2O

RX(8) RCT X 82544-17-0  
RGT AB 16853-85-3 LiAlH4  
PRO AA 108693-72-7  
SOL 109-99-9 THF

RX(12) RCT AA 108693-72-7, M 123-54-6  
RGT O 16872-11-0 HBF4  
PRO AG 160791-71-9  
SOL 75-09-2 CH2Cl2

RX(14) RCT AG 160791-71-9  
RGT F 302-01-2 N2H4  
PRO AI 160824-68-0  
SOL 64-17-5 EtOH

RX(23) RCT AV 160811-27-8

STAGE(1)  
RGT AS 7719-09-7 SOCl2

STAGE(2)  
SOL 109-99-9 THF

STAGE(3)  
RCT AI 160824-68-0  
SOL 109-99-9 THF

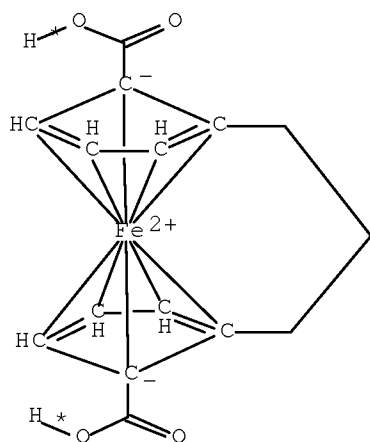
STAGE(4)  
RGT J 121-44-8 Et3N  
SOL 109-99-9 THF

PRO AX 160791-76-4

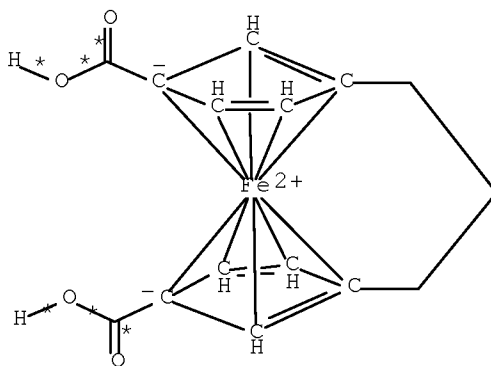
RX(163) OF 260 COMPOSED OF RX(7), RX(8), RX(12), RX(14), RX(25)

10/595943

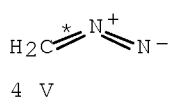
RX(163) T + U + 4 V + 2 M + 2 AQ ==> AZ



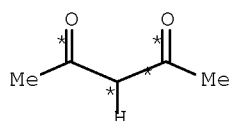
T



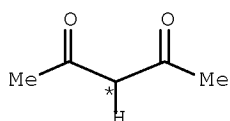
U



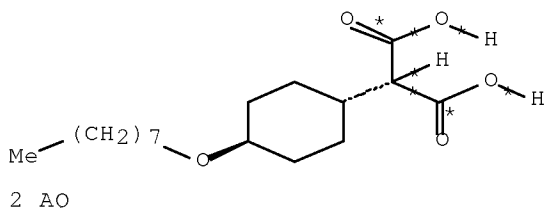
4 V



M



M



2 AQ

5  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(7) RCT T 155565-57-4, U 155565-58-5, V 334-88-3  
PRO W 82522-10-9, X 82544-17-0  
SOL 67-56-1 MeOH, 60-29-7 Et2O

RX(8) RCT X 82544-17-0  
RGT AB 16853-85-3 LiAlH4  
PRO AA 108693-72-7  
SOL 109-99-9 THF

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RX(12) RCT AA 108693-72-7, M 123-54-6  
 RGT O 16872-11-0 HBF4  
 PRO AG 160791-71-9  
 SOL 75-09-2 CH2Cl2

RX(14) RCT AG 160791-71-9  
 RGT F 302-01-2 N2H4  
 PRO AI 160824-68-0  
 SOL 64-17-5 EtOH

RX(25) RCT AQ 123854-20-6

STAGE(1)  
 RGT AS 7719-09-7 SOCl2

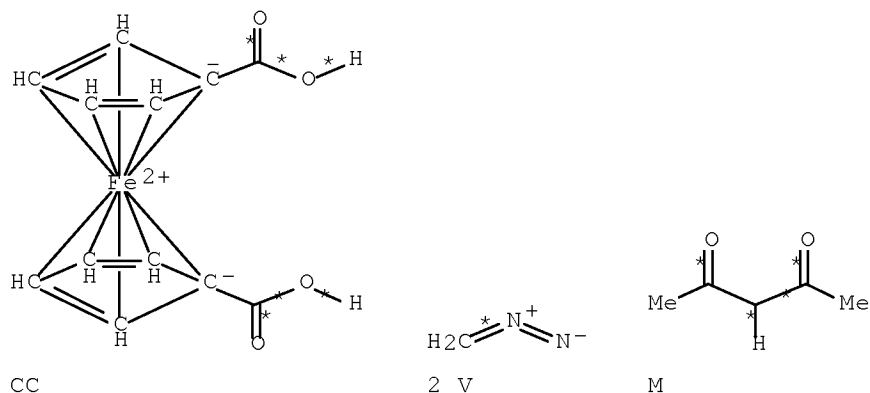
STAGE(2)  
 SOL 109-99-9 THF

STAGE(3)  
 RCT AI 160824-68-0  
 SOL 109-99-9 THF

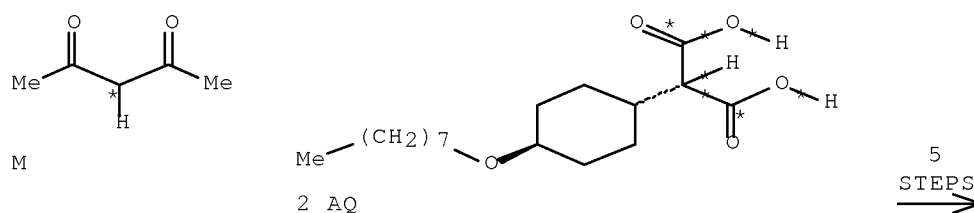
STAGE(4)  
 RGT J 121-44-8 Et3N  
 SOL 109-99-9 THF

PRO AZ 160791-78-6

RX(170) OF 260 COMPOSED OF RX(38), RX(9), RX(4), RX(5), RX(21)  
 RX(170) CC + 2 V + 2 M + 2 AQ ==> AU



10/595943



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(38) RCT CC 1293-87-4, V 334-88-3  
PRO AD 1273-95-6  
SOL 67-56-1 MeOH, 60-29-7 Et2O

RX(9) RCT AD 1273-95-6  
RGT AB 16853-85-3 LiAlH4  
PRO L 1291-48-1  
SOL 109-99-9 THF

RX(4) RCT L 1291-48-1, M 123-54-6  
RGT O 16872-11-0 HBF4  
PRO N 160791-68-4  
SOL 7732-18-5 Water

RX(5) RCT N 160791-68-4  
RGT F 302-01-2 N2H4  
PRO Q 160791-69-5  
SOL 64-17-5 EtOH

RX(21) RCT AQ 123854-20-6

STAGE(1)  
RGT AS 7719-09-7 SOCl2

STAGE(2)  
SOL 109-99-9 THF

STAGE(3)  
RCT Q 160791-69-5  
SOL 109-99-9 THF

STAGE(4)  
RGT J 121-44-8 Et3N  
SOL 109-99-9 THF

PRO AU 160824-73-7

L91 ANSWER 15 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 121:83144 CASREACT Full-text

TITLE: Studies on spiroheterocycles: Synthesis of new  
spiro-4-thiazolidinones as possible biodynamics

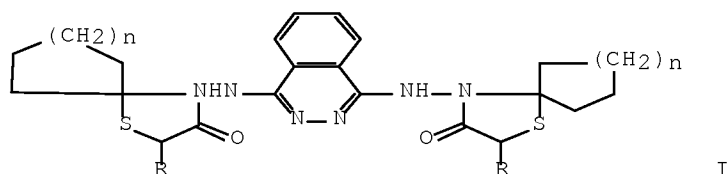
AUTHOR(S): Upadhyay, P.S.; Joshi, H.D.; Baxi, A.J.

CORPORATE SOURCE: Dep. Chem., Saurashtra Univ., Rajkot, 360 005, India



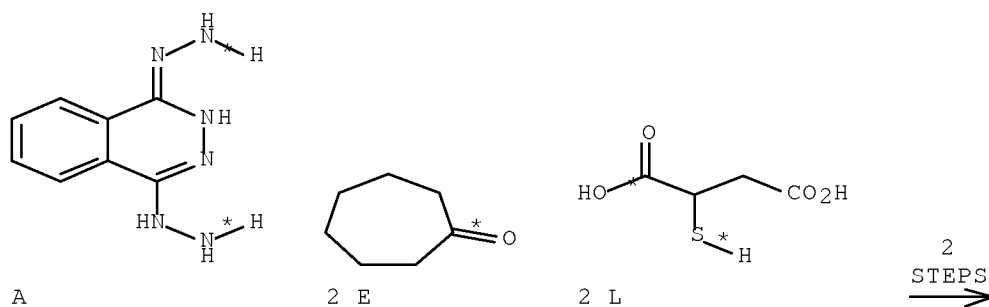
10/595943

SOURCE: Journal of Sciences, Islamic Republic of Iran (1992),  
3(1-2), 30-3  
CODEN: JSIIEN; ISSN: 1016-1104  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Spiro-4-thiazolidinones I (R = H, Me, CH<sub>2</sub>CO<sub>2</sub>H, n = 1,2,3,4) have been synthesized by the cyclocondensation of phthalazinyll hydrazones with cyclic ketones and substituted mercaptoacetic acids, HSCHRCO<sub>2</sub>H. Compds. were screened for their antibacterial, antifungal and antihypertensive activity. The combined elemental analyses and spectroscopic data prove the authenticity of the synthesized compds.

RX(8) OF 8 COMPOSED OF RX(2), RX(5)  
RX(8) A + 2 E + 2 L ==> M



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT A 484-23-1, E 502-42-1  
PRO F 156213-51-3  
SOL 64-17-5 EtOH  
  
RX(5) RCT F 156213-51-3, L 70-49-5  
RGT I 7646-85-7 ZnCl<sub>2</sub>  
PRO M 156213-63-7  
NTE thermal

L91 ANSWER 16 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 121:34970 CASREACT Full-text

TITLE: The cyclization of (Z)- and (E)-3-ethoxycarbonyl-4-(3'-chloro-6'-methylphenyl)-but-3-enoic acid and synthesis of polysubstituted naphthoic acid

AUTHOR(S): Mahmoud, M. R.

CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt

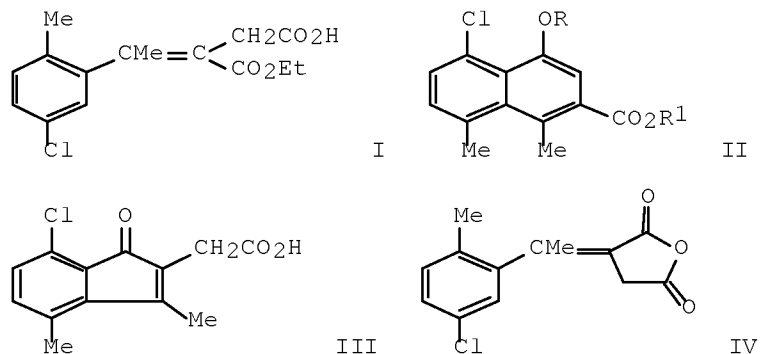
SOURCE: Journal of the Chemical Society of Pakistan (1993), 15(4), 247-51

CODEN: JCSPDF; ISSN: 0253-5106

DOCUMENT TYPE: Journal

LANGUAGE: English

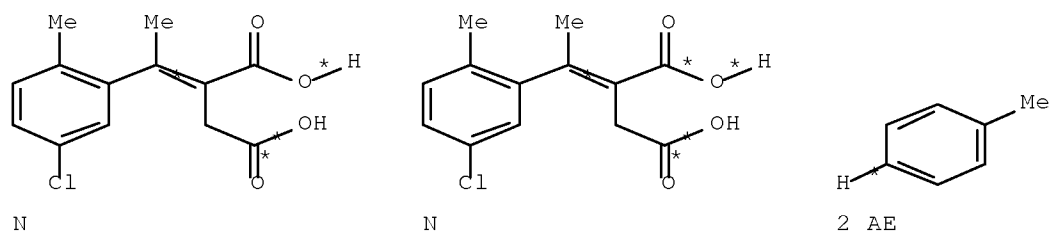
GI



AB Condensing 5-chloro-2-methylacetophenone with di-Et succinate in the presence of KOBu-t (Z)- and (E)-butenoate I. Cyclization of I with Ac<sub>2</sub>O gave naphthalene II (R = Ac, H, Me; R<sub>1</sub> = H, Me, Et) and oxoindenylic acid III via the anhydride IV, resp. The reactions of (E)-IV with aromatic hydrocarbons, amines and anhydrous AlCl<sub>3</sub> in Cl<sub>2</sub>CHCHCl<sub>2</sub> were also investigated.

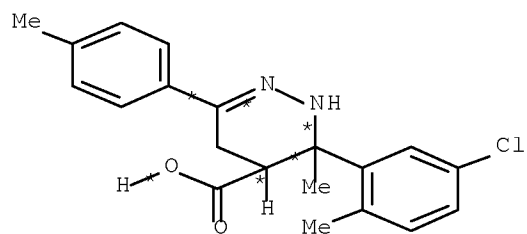
RX(54) OF 62 COMPOSED OF RX(5), RX(12), RX(14)

RX(54) 2 N + 2 AE ==&gt; AI + AJ

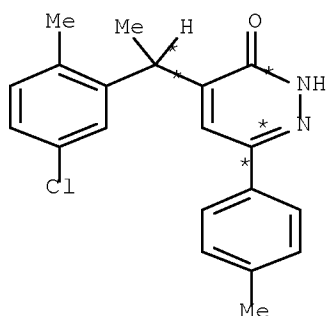


10/595943

3  
STEPS  
→



AI



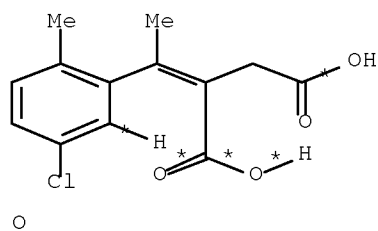
AJ

RX(5)      RCT    N 155651-98-2  
              RGT    R 538-75-0 DCC  
              PRO    J 155651-96-0  
              SOL    71-43-2 Benzene

RX(12)     RCT    J 155651-96-0, AE 108-88-3  
              RGT    L 7446-70-0 AlCl3  
              PRO    AF 155652-05-4  
              SOL    108-88-3 PhMe

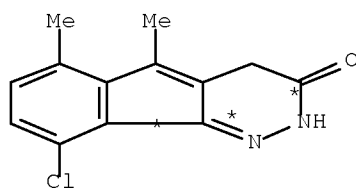
RX(14)     RCT    AF 155652-05-4  
              RGT    AK 302-01-2 N2H4  
              PRO    AI 155652-07-6, AJ 155652-08-7  
              SOL    71-36-3 BuOH

RX(56) OF 62 COMPOSED OF RX(6), RX(15), RX(16)  
 RX(56)      O    ==>    AN



O

3  
STEPS  
→



AN

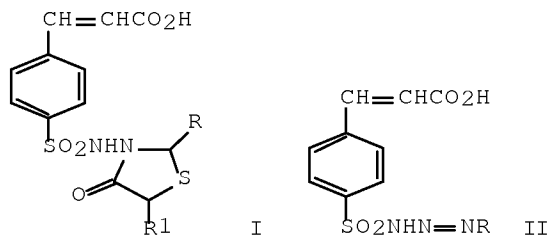
RX(6) RCT O 155651-99-3  
 RGT U 75-36-5 AcCl  
 PRO T 155652-09-8

RX(15) RCT T 155652-09-8  
 RGT L 7446-70-0 AlCl3  
 PRO AM 155652-10-1  
 SOL 79-34-5 Cl2HCCHCl2

RX(16) RCT AM 155652-10-1  
 RGT AK 302-01-2 N2H4  
 PRO AN 155652-12-3  
 SOL 71-36-3 BuOH

L91 ANSWER 17 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 117:251263 CASREACT Full-text  
 TITLE: Preparation and antimicrobial activity of  
 4-(2'-aryl-5'-H/methyl/carboxymethyl-4'-thiazolidinon-  
 3'-yl-aminosulfonyl)cinnamic acids  
 AUTHOR(S): Shah, K. C.; Baxi, A. J.  
 CORPORATE SOURCE: Dep. Chem., Saurashtra Univ., Rajkot, 360005, India  
 SOURCE: Indian Journal of Heterocyclic Chemistry (1992), 1(5),  
 253-8  
 CODEN: IJCHEI; ISSN: 0971-1627  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

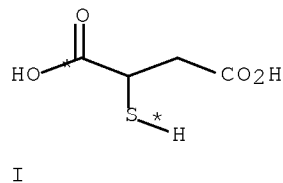
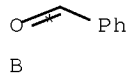
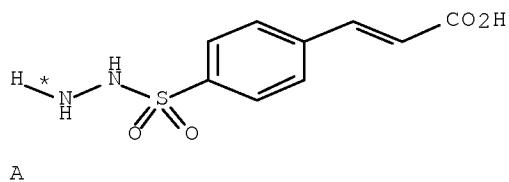


AB Title compds. I [R = Ph, p-(Me2N)C6H4, p-MeOC6H4, p-HOC6H4, o-HOC6H4, cinnamyl, 4-hydroxy-3-methoxyphenyl, 4-H2NC6H4, 3,4-dihydroxyphenyl, 2,4-dichlorophenyl, p-ClC6H4, 2,6-dichlorophenyl, m-O2NC6H4, o-MeOC6H4, m-MeOC6H4, o-ClC6H4, o-O2NC6H4, 3-H2NC6H4, 3,4-dichlorophenyl, 2-hydroxynaphthyl; R1 = H, Me, CH2CO2H] were prepared by the addition condensation of 4-benzalhydrazinosulfonylcinnamic acid II with thioglycolic acid, 2-mercaptopropionic acid and 2-mercaptosuccinic acid. The structures of the compds. have been confirmed by elemental analyses and spectral studies. The products have been screened for their antimicrobial activity.

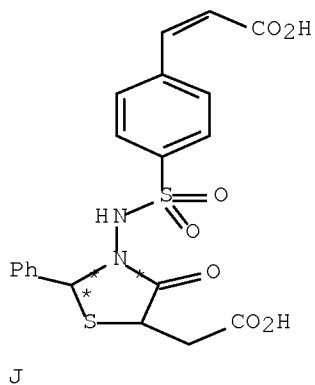
10/595943

RX(7) OF 7 COMPOSED OF RX(1), RX(4)

RX(7) A + B + I ==> J



2  
STEPS  
→



RX(1) RCT A 17641-31-5, B 100-52-7  
PRO C 143876-46-4  
SOL 123-91-1 Dioxane

RX(4) RCT C 143876-46-4, I 70-49-5  
RGT K 7645-85-7 ZnCl2  
PRO J 143877-02-5

L91 ANSWER 18 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 113:23664 CASREACT [Full-text](#)

TITLE: Benzophenanthridines. XI. Rodionov-Suvorov systems.  
Synthesis of the first example of  
11-aminobenzo[c]phenanthridines -  
11-amino-6-methyl-11,12-dihydrobenzo[c]phenanthridine

AUTHOR(S): Maslennikova, L. V.; Sladkov, V. I.; Suvorov, N. N.

CORPORATE SOURCE: USSR

10/595943

SOURCE:

Zhurnal Organicheskoi Khimii (1990), 26(2), 441-5

CODEN: ZORKAE; ISSN: 0514-7492

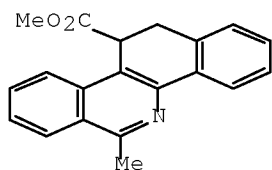
DOCUMENT TYPE:

Journal

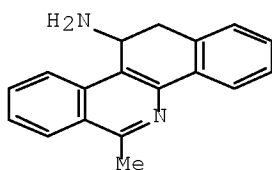
LANGUAGE:

Russian

GI



I

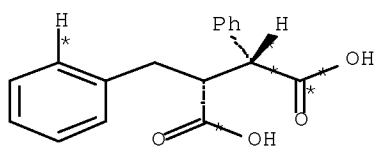


II

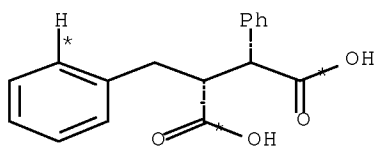
AB Me 6-methyl-11,12-dihydrobenzo[c]phenanthridine-11-carboxylate (I) was prepared from tri-Et 1,3-diphenyl-1,2,2-propanetricarboxylate via formation of erythro-1,3-diphenyl-1,2-propanedicarboxylic acid according to the AD → C → B Rodionov-Suvorov scheme in an 18% overall yield. Subsequent transformation of I to its hydrazide, azide, and isocyanate followed by Curtius rearrangement gave the title compound II.

RX(38) OF 55 COMPOSED OF RX(3), RX(2), RX(4), RX(5), RX(6), RX(7)

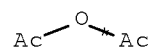
RX(38) 3 B + 3 O ==> V



B



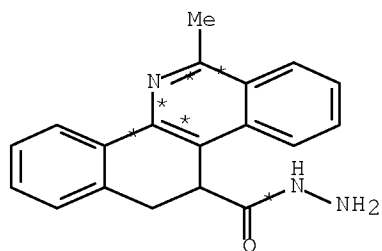
2 B



3 O

6  
STEPS  
→

10/595943



V  
YIELD 60%

RX(3) RCT B 56908-50-0  
RGT I 334-88-3 CH2N2  
PRO G 20972-45-6  
SOL 60-29-7 Et2O

RX(2) RCT G 20972-45-6  
PRO H 127845-14-1  
NTE polyphosphoric acid

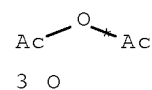
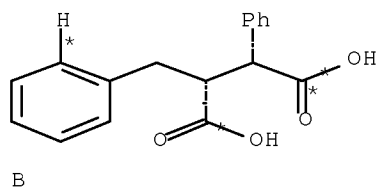
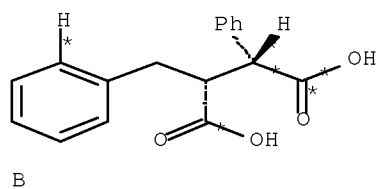
RX(4) RCT H 127845-14-1  
RGT M 5470-11-1 H2NOH-HCl  
PRO K 127845-15-2, L 127845-22-1  
SOL 110-86-1 Pyridine

RX(5) RCT K 127845-15-2, O 108-24-7  
RGT R 7772-99-8 SnCl2  
PRO P 127845-16-3, Q 127845-17-4  
SOL 108-24-7 Ac2O

RX(6) RCT Q 127845-17-4  
RGT T 10025-87-3 POC13  
PRO S 104958-38-5  
SOL 95-47-6 o-Xylene

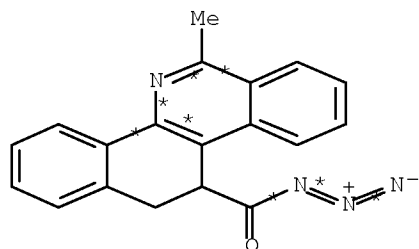
RX(7) RCT S 104958-38-5  
RGT W 302-01-2 N2H4  
PRO V 127845-19-6  
SOL 64-17-5 EtOH

RX(43) OF 55 COMPOSED OF RX(3), RX(2), RX(4), RX(5), RX(6), RX(7), RX(8)  
RX(43) 2 B + 3 O ==> Y



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7  
STEPS  
→



Y  
YIELD 74%

RX(3) RCT B 56908-50-0  
RGT I 334-88-3 CH2N2  
PRO G 20972-45-6  
SOL 60-29-7 Et2O

RX(2) RCT G 20972-45-6  
PRO H 127845-14-1  
NTE polyphosphoric acid

RX(4) RCT H 127845-14-1  
RGT M 5470-11-1 H2NOH-HCl  
PRO K 127845-15-2, L 127845-22-1  
SOL 110-86-1 Pyridine

RX(5) RCT K 127845-15-2, O 108-24-7  
RGT R 7772-99-8 SnCl2  
PRO P 127845-16-3, Q 127845-17-4  
SOL 108-24-7 Ac2O

RX(6) RCT Q 127845-17-4  
RGT T 10025-87-3 POC13  
PRO S 104958-38-5  
SOL 95-47-6 o-Xylene

RX(7) RCT S 104958-38-5  
RGT W 302-01-2 N2H4  
PRO V 127845-19-6  
SOL 64-17-5 EtOH

RX(8) RCT V 127845-19-6  
RGT Z 7632-00-0 NaNO2  
PRO Y 127845-20-9  
SOL 64-19-7 AcOH, 7732-18-5 Water

L91 ANSWER 19 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 112:207807 CASREACT Full-text

TITLE: N-aminophthalimide derivative-containing high-contrast dot-enhancing composition

INVENTOR(S): Kojima, Yasuhiko; Pilot, John; Waxman, Burton H.

PATENT ASSIGNEE(S): Polychrome Corp., USA; Dainippon Ink Chemical Industry Co.

SOURCE: U.S., 13 pp.



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CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

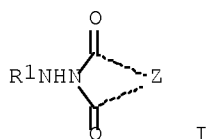
English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

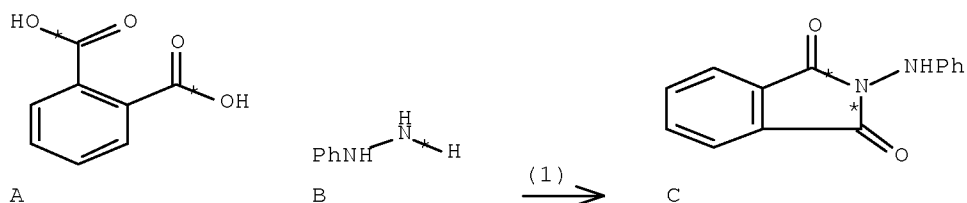
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4882261	A	19891121	US 1988-211980	19880627
JP 02052333	A	19900221	JP 1989-131228	19890524
AU 8936127	A	19900104	AU 1989-36127	19890607
AU 620101	B2	19920213		
EP 349274	A2	19900103	EP 1989-306523	19890627
EP 349274	A3	19900321		
EP 349274	B1	19940914		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
ES 2058532	T3	19941101	ES 1989-306523	19890627
CA 1335241	C	19950418	CA 1989-604005	19890627
			US 1988-211980	19880627

PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 112:207807  
GI

AB A dot-enhancing composition for use in a high-contrast neg.-working image-forming system contains a compound of the structure I (R1 = an aromatic group; Z = a substituted or unsubstituted aromatic nucleus, the 2 carbonyl groups are each bound to a different C atom of the aromatic nucleus). The composition, which may be incorporated into a lith Ag halide photog. emulsion, another hydrophilic colloid layer, a developer solution, or both, improves the d. and contrast of the images formed as well as provides harder, smoother, better formed dots for use in letterpress and offset lithog. plates.

RX(1) OF 1 A + B ==&gt; C



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RX(1) RCT A 88-99-3, B 100-63-0  
RGT D 7646-85-7 ZnCl2  
PRO C 4870-16-0

L91 ANSWER 20 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 110:75426 CASREACT Full-text

TITLE: Pyridazine derivatives. VI. Synthesis and hypotensive activity of 3-hydrazinothieno[2,3-h]cinnoline and its derivatives

AUTHOR(S): Garcia-Dominguez, Neftali; Ravina, Enrique; Santana, Lourdes; Teran, Carmen; Garcia-Mera, Gerardo; Orallo, Francisco; Crespo, Manuel; Fontenla, Jose Angel

CORPORATE SOURCE: Lab. Pharm. Chem., Univ. Santiago de Compostela, Spain

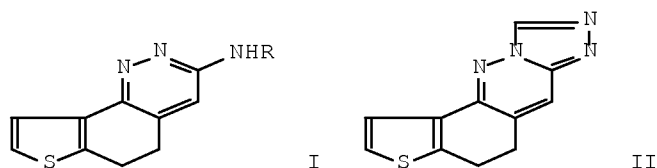
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1988), 321(10), 735-8

CODEN: ARPMAS; ISSN: 0365-6233

DOCUMENT TYPE: Journal

LANGUAGE: English

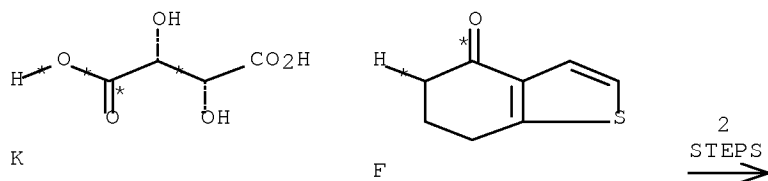
GI



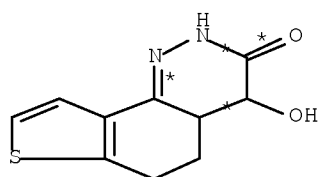
AB The title compound (I, R = NH<sub>2</sub>) was prepared from thiophene and succinic anhydride in 8 steps. Treatment of I (R = NH<sub>2</sub>) with HCO<sub>2</sub>H gave the triazolothienocinnoline II. I (R = NH<sub>2</sub>) had dose-dependent protracted antihypertensive activity which was significantly reduced in I (R = N:CM<sub>2</sub>). Cyclization to II eliminated the antihypertensive activity.

RX(14) OF 45 COMPOSED OF RX(3), RX(5)

RX(14) K + F ==> R



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R  
YIELD 92%

RX(3) RCT K 87-69-4

STAGE(1)

RGT H 7790-28-5 NaIO<sub>4</sub>, I 7664-93-9 H<sub>2</sub>SO<sub>4</sub>  
SOL 7732-18-5 Water

STAGE(2)

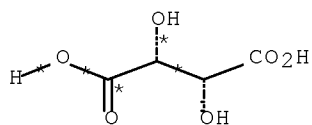
RCT F 13414-95-4  
RGT L 1310-73-2 NaOH  
SOL 64-17-5 EtOH

PRO G 118736-67-7

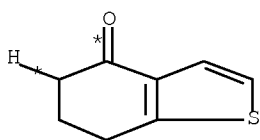
RX(5) RCT G 118736-67-7  
RGT C 302-01-2 N<sub>2</sub>H<sub>4</sub>  
PRO R 118736-68-8  
SOL 64-17-5 EtOH

RX(23) OF 45 COMPOSED OF RX(3), RX(5), RX(7)

RX(23) K + F ==> T

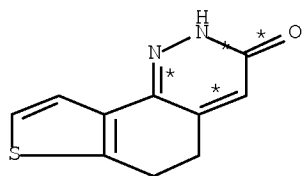


K



F

3  
STEPS  
→



T  
YIELD 65%

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RX(3) RCT K 87-69-4

STAGE(1)

RGT H 7790-28-5 NaIO<sub>4</sub>, I 7664-93-9 H<sub>2</sub>SO<sub>4</sub>  
SOL 7732-18-5 Water

STAGE(2)

RCT F 13414-95-4  
RGT L 1310-73-2 NaOH  
SOL 64-17-5 EtOH

PRO G 118736-67-7

RX(5) RCT G 118736-67-7  
RGT C 302-01-2 N<sub>2</sub>H<sub>4</sub>  
PRO R 118736-68-8  
SOL 64-17-5 EtOH

RX(7) RCT R 118736-68-8  
RGT U 127-68-4 m-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>Na, L 1310-73-2 NaOH  
PRO T 118777-73-4  
SOL 7732-18-5 Water

L91 ANSWER 21 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 108:111649 CASREACT Full-text

TITLE: Microenvironmental effects of water-soluble polymers  
on the chemiluminescence of luminol and its analogs

AUTHOR(S): Karatani, Hajime

CORPORATE SOURCE: Fac. Text. Sci., Kyoto Inst. Technol., Kyoto, 606,  
Japan

SOURCE: Bulletin of the Chemical Society of Japan (1987),  
60(6), 2023-9

CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE: Journal

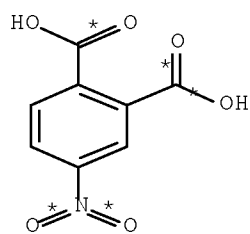
LANGUAGE: English

AB The effects of water-soluble polymers (WSPs), such as bovine serum albumin (BSA) and poly(ethylenimine) on chemiluminescence (CL) in an aqueous solution have been studied. The CL emission, particularly in the initial stage of the CL reaction, was strongly enhanced by increasing the concns. of these WSPs. This was attributed to the acceleration of the chemical reactions prior to the formation of the light-emitting species. BSA was also peculiar in that it could enhance CL under neutral pH conditions. It was suggested that these WSPs offered hydrophobic and basic microenvironments well suited to the CL reaction.

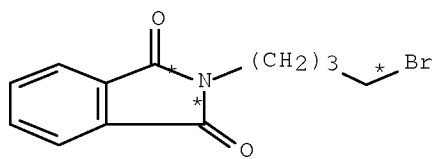
RX(60) OF 100 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(6)

RX(60) A + H ==> K

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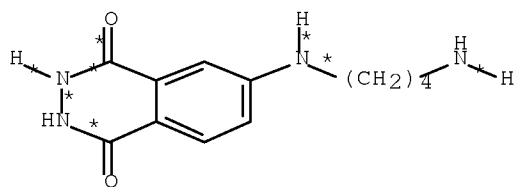


A



H

5  
STEPS  
→

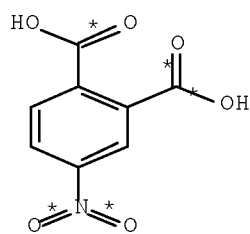


K

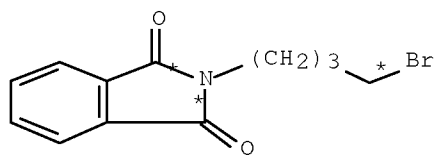
RX(1)	RCT	A	610-27-5
	PRO	B	5466-84-2
RX(2)	RCT	B	5466-84-2
	PRO	C	41663-84-7
RX(3)	RCT	C	41663-84-7
	RGT	E	7647-01-0 HCl, F 7772-99-8 SnCl2
	PRO	D	2307-00-8
	SOL		7732-18-5 Water
RX(4)	RCT	H	5394-18-3, D 2307-00-8
	PRO	I	73819-85-9
RX(6)	RCT	I	73819-85-9
	RGT	L	302-01-2 N2H4
	PRO	K	66612-28-0
	SOL		64-17-5 EtOH

RX(70) OF 100 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(11), RX(7)  
 RX(70) A + H + V ==> O

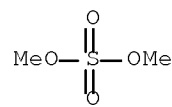
10/595943



A

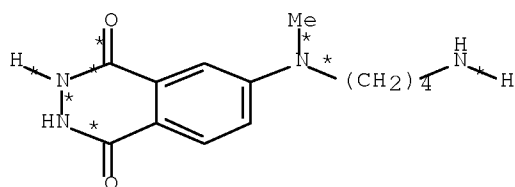


H



V

6  
STEPS  
→



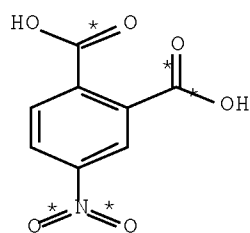
O

RX(1)	RCT	A 610-27-5
	PRO	B 5466-84-2
RX(2)	RCT	B 5466-84-2
	PRO	C 41663-84-7
RX(3)	RCT	C 41663-84-7
	RGT	E 7647-01-0 HCl, F 7772-99-8 SnCl2
	PRO	D 2307-00-8
	SOL	7732-18-5 Water
RX(4)	RCT	H 5394-18-3, D 2307-00-8
	PRO	I 73819-85-9
RX(11)	RCT	I 73819-85-9, V 77-78-1
	PRO	N 113120-83-5
RX(7)	RCT	N 113120-83-5
	RGT	L 302-01-2 N2H4
	PRO	O 80944-69-0
	SOL	64-17-5 EtOH

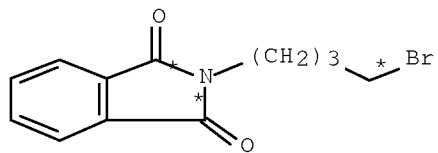
RX(71) OF 100 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(12), RX(8)

10/595943

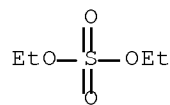
RX(71)      A   +   H   +   W   ==>   Q



A

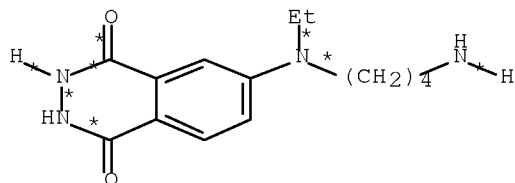


H



W

6  
STEPS  
→



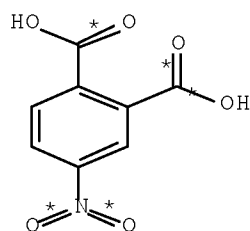
Q

RX(1)	RCT	A	610-27-5
	PRO	B	5466-84-2
RX(2)	RCT	B	5466-84-2
	PRO	C	41663-84-7
RX(3)	RCT	C	41663-84-7
	RGT	E	7647-01-0 HCl, F 7772-99-8 SnCl2
	PRO	D	2307-00-8
	SOL	7732-18-5	Water
RX(4)	RCT	H	5394-18-3, D 2307-00-8
	PRO	I	73819-85-9
RX(12)	RCT	I	73819-85-9, W 64-67-5
	PRO	P	73819-87-1
RX(8)	RCT	P	73819-87-1
	RGT	L	302-01-2 N2H4
	PRO	Q	66612-29-1
	SOL	64-17-5	EtOH

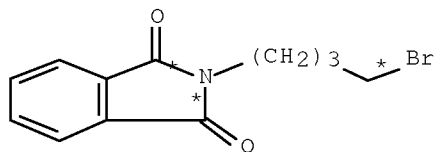
10/595943

RX(72) OF 100 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(13), RX(9)

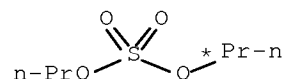
RX(72) A + H + X ==> S



A

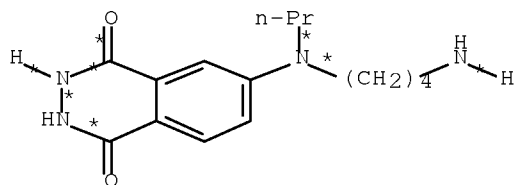


H



X

6  
STEPS  
→



S

RX(1)	RCT	A 610-27-5
	PRO	B 5466-84-2
RX(2)	RCT	B 5466-84-2
	PRO	C 41663-84-7
RX(3)	RCT	C 41663-84-7
	RGT	E 7647-01-0 HCl, F 7772-99-8 SnCl2
	PRO	D 2307-00-8
	SOL	7732-18-5 Water
RX(4)	RCT	H 5394-18-3, D 2307-00-8
	PRO	I 73819-85-9
RX(13)	RCT	I 73819-85-9, X 598-05-0
	PRO	R 113120-84-6
RX(9)	RCT	R 113120-84-6
	RGT	L 302-01-2 N2H4
	PRO	S 113120-81-3

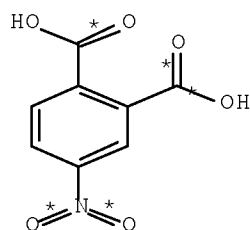


10/595943

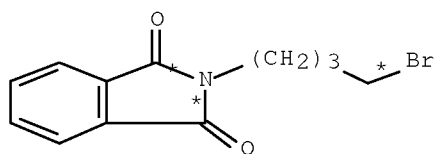
SOL 64-17-5 EtOH

RX(73) OF 100 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(14), RX(10)

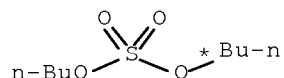
RX(73) A + H + Y ==> U



A

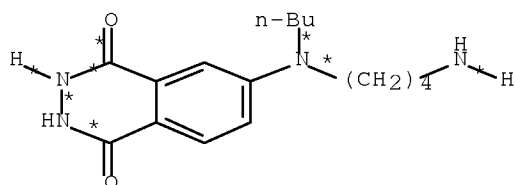


H



Y

6  
STEPS  
→



U

RX(1)	RCT	A 610-27-5
	PRO	B 5466-84-2
RX(2)	RCT	B 5466-84-2
	PRO	C 41663-84-7
RX(3)	RCT	C 41663-84-7
	RGT	E 7647-01-0 HCl, F 7772-99-8 SnCl2
	PRO	D 2307-00-8
	SOL	7732-18-5 Water
RX(4)	RCT	H 5394-18-3, D 2307-00-8
	PRO	I 73819-85-9
RX(14)	RCT	I 73819-85-9, Y 625-22-9
	PRO	T 113120-85-7
RX(10)	RCT	T 113120-85-7

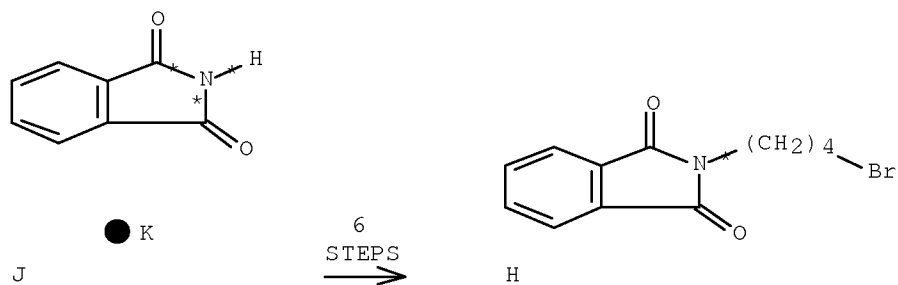
10/595943

RGT L 302-01-2 N2H4  
 PRO U 113120-02-4  
 SOL 64-17-5 EtOH

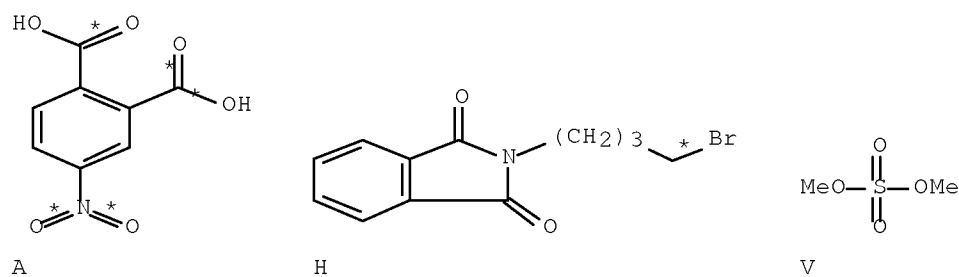
RX(92) OF 100 COMPOSED OF REACTION SEQUENCE RX(5), RX(4), RX(11), RX(7)  
 AND REACTION SEQUENCE RX(1), RX(2), RX(3), RX(4), RX(11), RX(7)

...J ==> H...

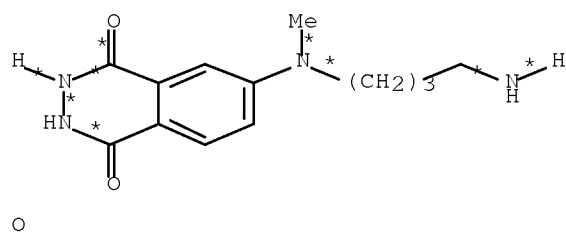
... A + H + V ==> O



START NEXT REACTION SEQUENCE



6  
 STEPS  
 →



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RX(5) RCT J 1074-82-4  
 PRO H 5394-18-3

RX(1) RCT A 610-27-5  
 PRO B 5466-84-2

RX(2) RCT B 5466-84-2  
 PRO C 41663-84-7

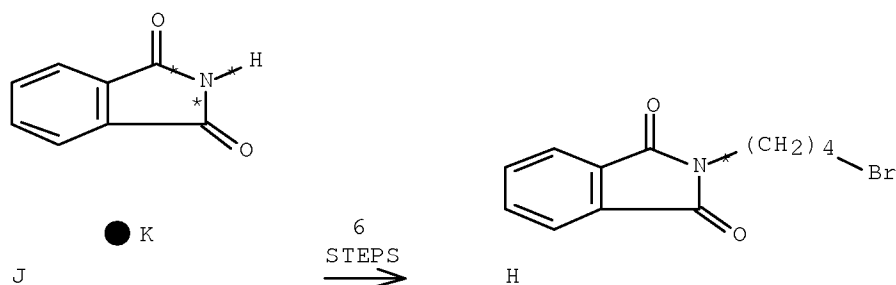
RX(3) RCT C 41663-84-7  
 RGT E 7647-01-0 HCl, F 7772-99-8 SnCl2  
 PRO D 2307-00-8  
 SOL 7732-18-5 Water

RX(4) RCT H 5394-18-3, D 2307-00-8  
 PRO I 73819-85-9

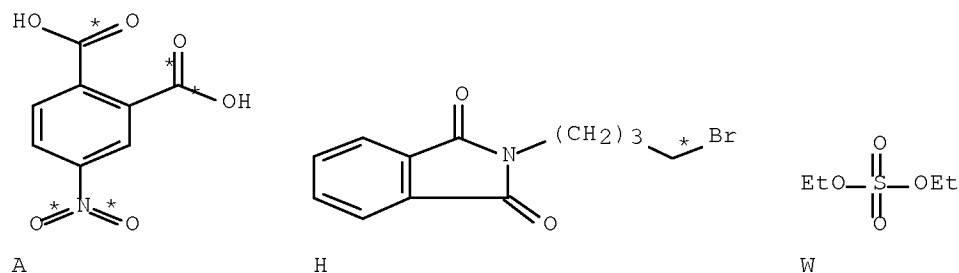
RX(11) RCT I 73819-85-9, V 77-78-1  
 PRO N 113120-83-5

RX(7) RCT N 113120-83-5  
 RGT L 302-01-2 N2H4  
 PRO O 80944-69-0  
 SOL 64-17-5 EtOH

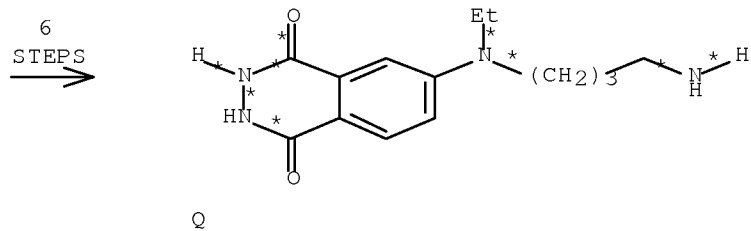
RX(93) OF 100 COMPOSED OF REACTION SEQUENCE RX(5), RX(4), RX(12), RX(8)  
 AND REACTION SEQUENCE RX(1), RX(2), RX(3), RX(4), RX(12), RX(8)  
 ...J ==> H...  
 ... A + H + W ==> Q



START NEXT REACTION SEQUENCE



10/595943



RX(5) RCT J 1074-82-4  
PRO H 5394-18-3

RX(1) RCT A 610-27-5  
PRO B 5466-84-2

RX(2) RCT B 5466-84-2  
PRO C 41663-84-7

RX(3) RCT C 41663-84-7  
RGT E 7647-01-0 HCl, F 7772-99-8 SnCl2  
PRO D 2307-00-8  
SOL 7732-18-5 Water

RX(4) RCT H 5394-18-3, D 2307-00-8  
PRO I 73819-85-9

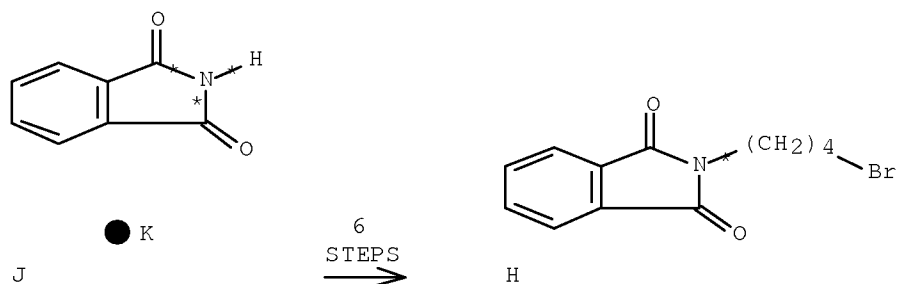
RX(12) RCT I 73819-85-9, W 64-67-5  
PRO P 73819-87-1

RX(8) RCT P 73819-87-1  
RGT L 302-01-2 N2H4  
PRO Q 66612-29-1  
SOL 64-17-5 EtOH

RX(94) OF 100 COMPOSED OF REACTION SEQUENCE RX(5), RX(4), RX(13), RX(9)  
AND REACTION SEQUENCE RX(1), RX(2), RX(3), RX(4), RX(13), RX(9)

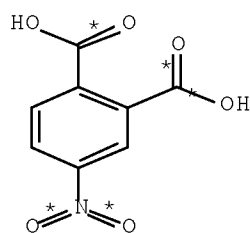
...J ==> H...

... A + H + X ==> S

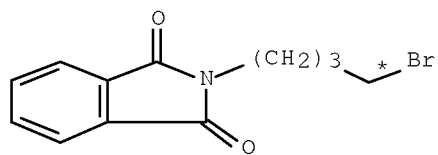


10/595943

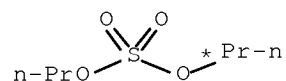
START NEXT REACTION SEQUENCE



A

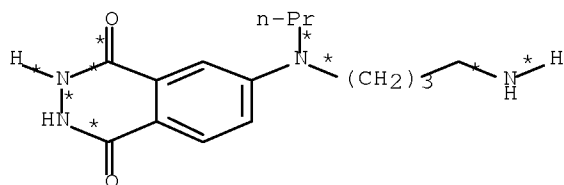


H



X

6  
STEPS  
→



S

RX(5)	RCT	J	1074-82-4
	PRO	H	5394-18-3
RX(1)	RCT	A	610-27-5
	PRO	B	5466-84-2
RX(2)	RCT	B	5466-84-2
	PRO	C	41663-84-7
RX(3)	RCT	C	41663-84-7
	RGT	E	7647-01-0 HCl, F 7772-99-8 SnCl2
	PRO	D	2307-00-8
	SOL		7732-18-5 Water
RX(4)	RCT	H	5394-18-3, D 2307-00-8
	PRO	I	73819-85-9
RX(13)	RCT	I	73819-85-9, X 598-05-0
	PRO	R	113120-84-6
RX(9)	RCT	R	113120-84-6
	RGT	L	302-01-2 N2H4

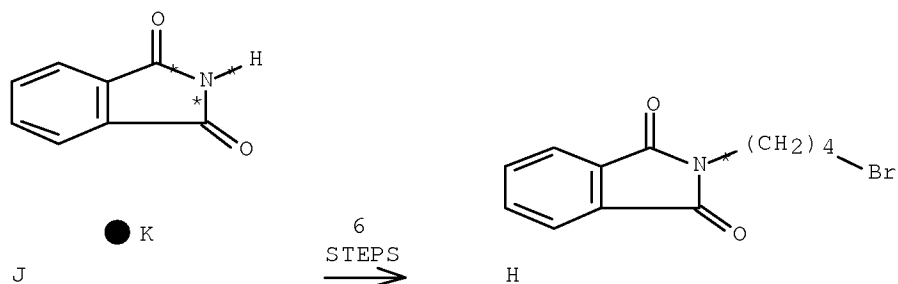
10/595943

PRO S 113120-81-3  
SOL 64-17-5 EtOH

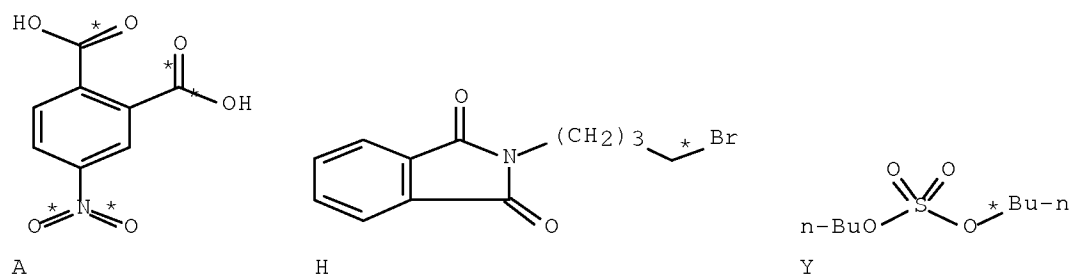
RX(95) OF 100 COMPOSED OF REACTION SEQUENCE RX(5), RX(4), RX(14), RX(10)  
AND REACTION SEQUENCE RX(1), RX(2), RX(3), RX(4), RX(14), RX(10)

...J ==> H...

... A + H + Y ==> U



START NEXT REACTION SEQUENCE



RX(5) RCT J 1074-82-4  
PRO H 5394-18-3

RX(1) RCT A 610-27-5  
PRO B 5466-84-2

RX(2) RCT B 5466-84-2  
PRO C 41663-84-7

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RX(3) RCT C 41663-84-7  
RGT E 7647-01-0 HCl, F 7772-99-8 SnCl2  
PRO D 2307-00-8  
SOL 7732-18-5 Water

RX(4) RCT H 5394-18-3, D 2307-00-8  
PRO I 73819-85-9

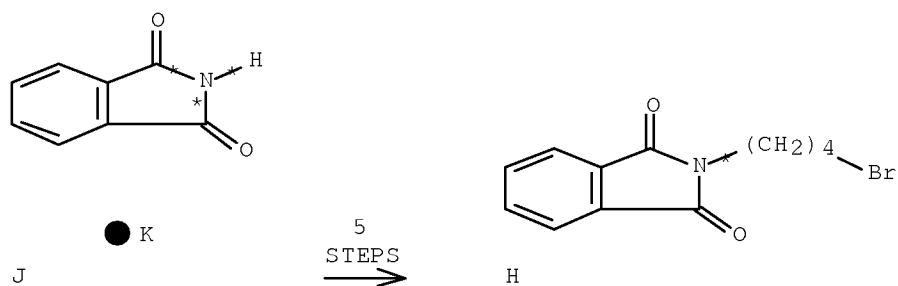
RX(14) RCT I 73819-85-9, Y 625-22-9  
PRO T 113120-85-7

RX(10) RCT T 113120-85-7  
RGT L 302-01-2 N2H4  
PRO U 113120-82-4  
SOL 64-17-5 EtOH

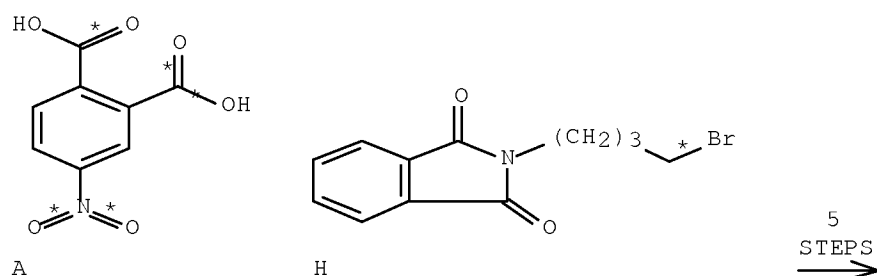
RX(96) OF 100 COMPOSED OF REACTION SEQUENCE RX(5), RX(4), RX(6)  
AND REACTION SEQUENCE RX(1), RX(2), RX(3), RX(4), RX(6)

...J ==> H...

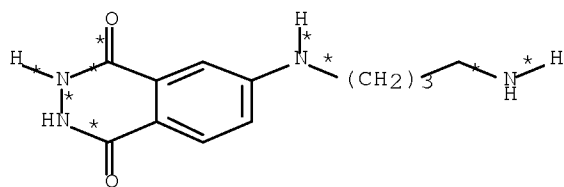
... A + H ==> K



START NEXT REACTION SEQUENCE



10/595943



RX(5) RCT J 1074-82-4  
PRO H 5394-18-3

RX(1) RCT A 610-27-5  
PRO B 5466-84-2

RX(2) RCT B 5466-84-2  
PRO C 41663-84-7

RX(3) RCT C 41663-84-7  
RGT E 7647-01-0 HCl, F 7772-99-8 SnCl2  
PRO D 2307-00-8  
SOL 7732-18-5 Water

RX(4) RCT H 5394-18-3, D 2307-00-8  
PRO I 73819-85-9

RX(6) RCT I 73819-85-9  
RGT L 302-01-2 N2H4  
PRO K 66612-28-0  
SOL 64-17-5 EtOH

L91 ANSWER 22 OF 30 CASREACT COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 108:21627 CASREACT Full-text  
TITLE: Use of 2-( $\alpha$ -naphthylethyl)furan in diene  
synthesis: an access to the derivatives of original  
heterocycles  
AUTHOR(S): Duval, O.; Gomes, L. Mavoungou  
CORPORATE SOURCE: Lab. Chim. Org., Univ. Angers, Angers, 49000, Fr.  
SOURCE: Bulletin de la Societe Chimique de France (1987), (1),  
131-42  
CODEN: BSCFAS; ISSN: 0037-8968  
DOCUMENT TYPE: Journal  
LANGUAGE: French  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Naphthyl Et furandicarboxylic acids (e.g., I, R = PhCH2CH2,  $\alpha$ -naphthyl ethyl) were prepared and converted to new heterocycles that include dihydrooxonaphthocycloheptafuran II, dioxotetrahydrobenzonaphthodicycloheptafuran III, and

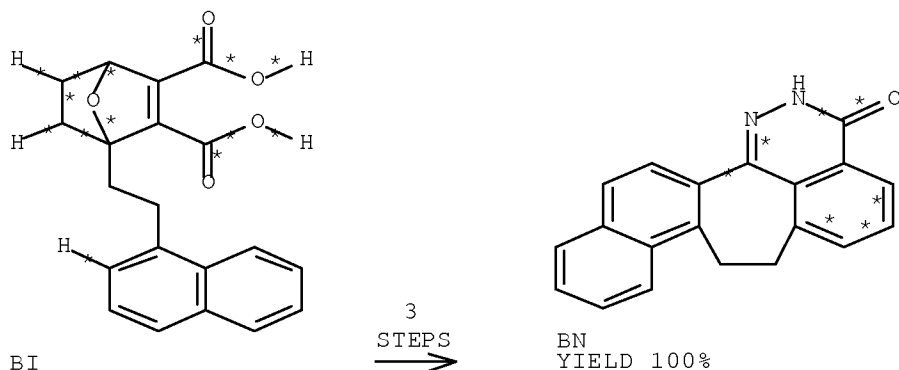


10/595943

dioxotetrahydrodinaphthodicycloheptafuran IV. A number of dihydronaphthocycloheptaphthalazines, e.g., V, prepared in connection with this study, are also described.

RX(172) OF 364 COMPOSED OF RX(26), RX(27), RX(28)

RX(172) BI ==> BN



RX(26) RCT BI 112036-40-5  
RGT AQ 7664-38-2 H3PO4  
PRO BJ 112036-41-6  
SOL 64-19-7 AcOH

RX(27) RCT BJ 112036-41-6  
RGT BL 7446-70-0 AlCl3, BC 7726-95-6 Br2  
PRO BK 112036-42-7  
SOL 79-34-5 Cl2HCCHCl2

RX(28) RCT BK 112036-42-7  
RGT S 302-01-2 N2H4  
PRO BN 112036-43-8  
SOL 64-19-7 AcOH

L91 ANSWER 23 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 105:172383 CASREACT Full-text

TITLE: Conformationally restricted congeners of hypotensive and platelet aggregation inhibitors:  
6-aryl-5-methyl-4,5-dihydro-3(2H)-pyridazinones  
derived from 5H-indeno[1,2-c]pyridazine

AUTHOR(S): Cignarella, Giorgio; Barlocco, Daniela; Pinna, Gerard A.; Loriga, Mario; Tofanetti, Odoardo; Germini, Mauro; Sala, Franca

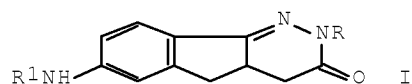
CORPORATE SOURCE: Ist. Chim. Farm. Tossicol., Univ. Milano, Milan, 20131, Italy

SOURCE: Journal of Medicinal Chemistry (1986), 29(11), 2191-4  
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

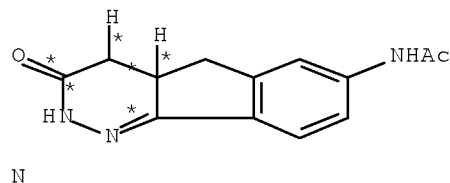
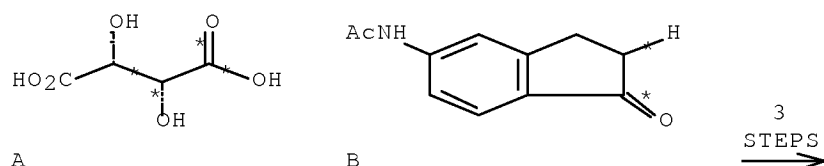
LANGUAGE: English

GI



AB Indeno[1,2-c]pyridazin-3-ones I ( $R = H, Me$ ;  $R_1 = H, Ac, COCHClMe$ ) were prepared as rigid congeners of hypotensive 6-aryl-5-methyl-4,5-dihydro-3(2H)-pyridazinones and tested as antihypertensive, antithrombotic, antiulcer, and antiinflammatory agents. Unlike the previously described 7-cyano derivative, which displayed only antiinflammatory action, the new series exhibited significant antihypertensive and antithrombotic properties. I ( $R = H, R_1 = H, Ac$ ) were found to be the most potent and long lasting in reducing the blood pressure in spontaneously hypertensive rats and in protecting mice from the induction of thrombosis. (ED<sub>50</sub> 2.60) I also exhibited antiinflammatory activity; and were highly effective in inhibiting indomethacin-induced ulcers in the rat.

RX(18) OF 26 COMPOSED OF RX(1), RX(2), RX(4)  
 RX(18) A + B ==> N



RX(1) RCT A 87-69-4

STAGE(1)

RGT D 7664-93-9 H<sub>2</sub>SO<sub>4</sub>, E 7790-28-5 NaIO<sub>4</sub>  
 SOL 7732-18-5 Water

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STAGE(2)

RCT B 58161-35-6  
RGT F 1310-73-2 NaOH  
SOL 64-17-5 EtOH

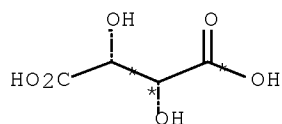
PRO C 103602-84-2

RX(2) RCT C 103602-84-2  
RGT J 7440-66-6 Zn  
PRO I 103422-85-1  
SOL 64-19-7 AcOH

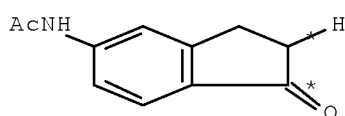
RX(4) RCT I 103422-85-1  
RGT O 302-01-2 N2H4  
PRO N 103422-54-4  
SOL 64-17-5 EtOH

RX(19) OF 26 COMPOSED OF RX(1), RX(2), RX(7)

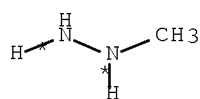
RX(19) A + B + T ==> U



A

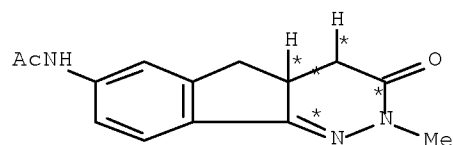


B



T

3  
STEPS  
→



U

RX(1) RCT A 87-69-4

STAGE(1)

RGT D 7664-93-9 H2SO4, E 7790-28-5 NaIO4  
SOL 7732-18-5 Water

STAGE(2)

RCT B 58161-35-6  
RGT F 1310-73-2 NaOH  
SOL 64-17-5 EtOH

PRO C 103602-84-2

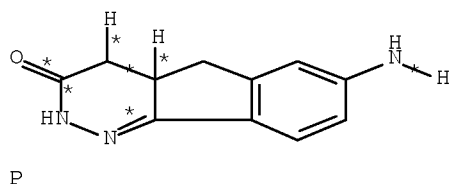
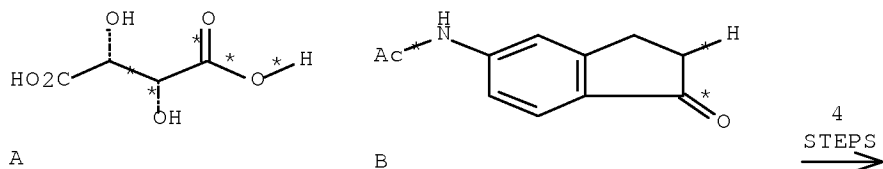
RX(2) RCT C 103602-84-2  
RGT J 7440-66-6 Zn

10/595943

PRO I 103422-85-1  
SOL 64-19-7 AcOH

RX(7) RCT I 103422-85-1, T 60-34-4  
PRO U 103794-15-6  
SOL 64-17-5 EtOH

RX(22) OF 26 COMPOSED OF RX(1), RX(2), RX(3), RX(5)  
RX(22) A + B ==> P



RX(1) RCT A 87-69-4

STAGE(1)

RGT D 7664-93-9 H2SO4, E 7790-28-5 NaIO4  
SOL 7732-18-5 Water

STAGE(2)

RCT B 58161-35-6  
RGT F 1310-73-2 NaOH  
SOL 64-17-5 EtOH

PRO C 103602-84-2

RX(2) RCT C 103602-84-2  
RGT J 7440-66-6 Zn  
PRO I 103422-85-1  
SOL 64-19-7 AcOH

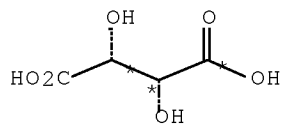
RX(3) RCT I 103422-85-1  
RGT M 7647-01-0 HCl  
PRO L 103422-62-4  
SOL 7647-01-0 HCl, 7732-18-5 Water

RX(5) RCT L 103422-62-4  
RGT O 302-01-2 N2H4

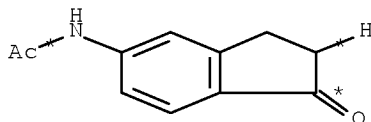
10/595943

PRO P 103422-53-3  
SOL 64-17-5 EtOH

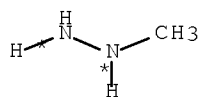
RX(23) OF 26 COMPOSED OF RX(1), RX(2), RX(3), RX(8)  
RX(23) A + B + T ==> V



A

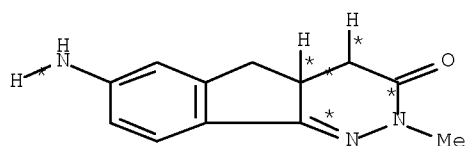


B



T

4  
STEPS  
→



V

RX(1) RCT A 87-69-4

STAGE(1)

RGT D 7664-93-9 H2SO4, E 7790-28-5 NaIO4  
SOL 7732-18-5 Water

STAGE(2)

RCT B 58161-35-6  
RGT F 1310-73-2 NaOH  
SOL 64-17-5 EtOH

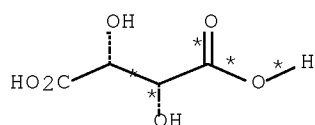
PRO C 103602-84-2

RX(2) RCT C 103602-84-2  
RGT J 7440-66-6 Zn  
PRO I 103422-85-1  
SOL 64-19-7 AcOH

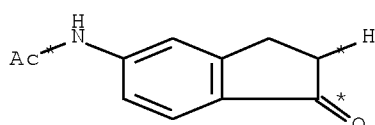
RX(3) RCT I 103422-85-1  
RGT M 7647-01-0 HCl  
PRO L 103422-62-4  
SOL 7647-01-0 HCl, 7732-18-5 Water

RX(8) RCT L 103422-62-4, T 60-34-4  
PRO V 103794-16-7  
SOL 64-17-5 EtOH

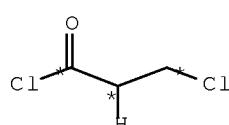
RX(26) OF 26 COMPOSED OF RX(1), RX(2), RX(3), RX(5), RX(6)  
RX(26) A + B + Q ==> R



A

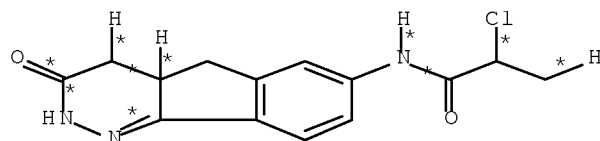


B



Q

5  
STEPS  
→



R

RX(1) RCT A 87-69-4

STAGE(1)  
RGT D 7664-93-9 H2SO4, E 7790-28-5 NaIO4  
SOL 7732-18-5 Water

STAGE(2)  
RCT B 58161-35-6  
RGT F 1310-73-2 NaOH  
SOL 64-17-5 EtOH

PRO C 103602-84-2

RX(2) RCT C 103602-84-2  
RGT J 7440-66-6 Zn  
PRO I 103422-85-1  
SOL 64-19-7 AcOH

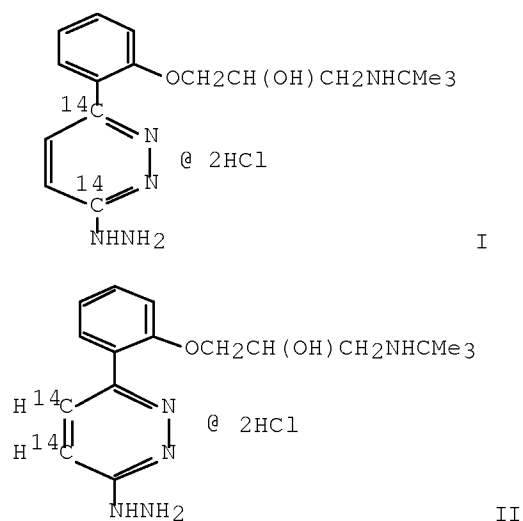
RX(3) RCT I 103422-85-1  
RGT M 7647-01-0 HCl  
PRO L 103422-62-4  
SOL 7647-01-0 HCl, 7732-18-5 Water

RX(5) RCT L 103422-62-4  
RGT O 302-01-2 N2H4  
PRO P 103422-53-3  
SOL 64-17-5 EtOH

RX(6) RCT P 103422-53-3, Q 625-36-5  
PRO R 103602-83-1  
SOL 108-88-3 PhMe

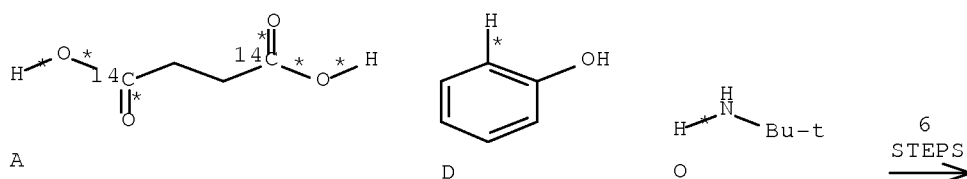
10/595943

TITLE: Syntheses of carbon-14-labeled prizidilol dihydrochloride  
 AUTHOR(S): Saunders, D.; Warrington, B. H.  
 CORPORATE SOURCE: Smith Kline and French Res. Ltd., Welwyn/Hertfordshire, AL6 9AR, UK  
 SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1985), 22(9), 869-81  
 CODEN: JLCRD4; ISSN: 0362-4803  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

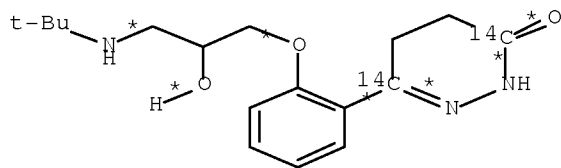


AB Two syntheses of radiolabeled prizidilol-2HCl are described. A ten-stage synthesis gave [3,6-<sup>14</sup>C<sub>2</sub>]prizidilol-2HCl I in an overall yield of 0.91%. A later, alternative procedure led to [4,5-<sup>14</sup>C<sub>2</sub>]prizidilol-2HCl II with an overall radiochem. yield of 8%.

RX(71) OF 111 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6)  
 RX(71) A + D + O ==> Q



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 $\Omega$ 

RX(1)        RCT    A 13613-74-6  
              RGT    C 7719-09-7 SOC12  
              PRO    B 42415-11-2

```

RX(2)      RCT  B 42415-11-2, D 108-95-2
           RGT  F 7446-70-0 AlCl3
           PRO  E 103912-99-8
           SOL  79-34-5 Cl2HCCHCl2

```

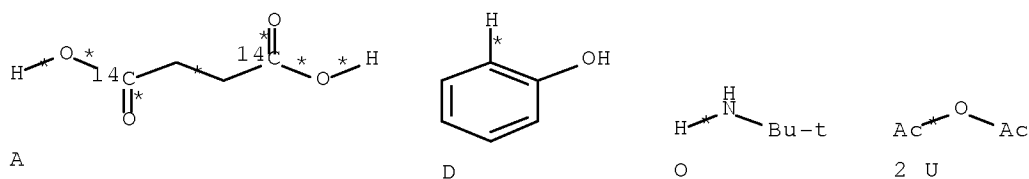
RX (3)	RCT	E	103912-99-8
	RGT	I	7647-01-0 HCl
	PRO	H	103913-00-4
	SOL		67-56-1 MeOH

RX(4)	RCT	H	103913-00-4	
	RGT	L	584-08-7 K2CO3,	M 3132-64-7 Epibromohydrin
	PRO	K	103913-01-5	
	SOL		78-93-3 EtCOMe	

RX(5)	RCT	K 103913-01-5, O 75-64-9
	PRO	P 103913-02-6
	SOL	67-56-1 MeOH

RX(6)	RCT	P 103913-02-6
	RGT	R 302-01-2 N2H4
	PRO	Q 103913-03-7
	SOL	64-19-7 AcOH, 7732-18-5 Water

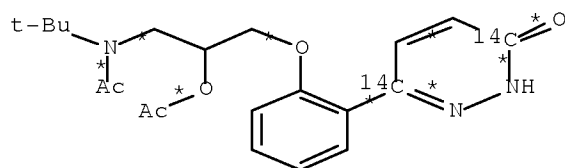
RX(74) OF 111 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(7)

$$\text{RX (74)} \quad \text{A} + \text{D} + \text{O} + 2 \text{U} \implies \text{V}$$




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7  
STEPS  
→



V

RX(1) RCT A 13613-74-6  
RGT C 7719-09-7 SOCl2  
PRO B 42415-11-2

RX(2) RCT B 42415-11-2, D 108-95-2  
RGT F 7446-70-0 AlCl3  
PRO E 103912-99-8  
SOL 79-34-5 Cl2HCCHCl2

RX(3) RCT E 103912-99-8  
RGT I 7647-01-0 HCl  
PRO H 103913-00-4  
SOL 67-56-1 MeOH

RX(4) RCT H 103913-00-4  
RGT L 584-08-7 K2CO3, M 3132-64-7 Epibromohydrin  
PRO K 103913-01-5  
SOL 78-93-3 EtCOMe

RX(5) RCT K 103913-01-5, O 75-64-9  
PRO P 103913-02-6  
SOL 67-56-1 MeOH

RX(6) RCT P 103913-02-6  
RGT R 302-01-2 N2H4  
PRO Q 103913-03-7  
SOL 64-19-7 AcOH, 7732-18-5 Water

RX(7) RCT Q 103913-03-7, U 108-24-7

STAGE(1)

RGT L 584-08-7 K2CO3

STAGE(2)

RGT W 7726-95-6 Br2

SOL 64-19-7 AcOH

PRO V 103913-04-8

L91 ANSWER 25 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 105:78865 CASREACT Full-text

TITLE: Studies on isoniazid derivatives. Preparation and antimicrobial activity of 2-aryl-3-(pyridylcarbonyl)-5-carboxymethyl-4-thiazolidinones

AUTHOR(S): Shah, R. R.; Mehta, R. D.; Parikh, A. R.

10/595943

CORPORATE SOURCE:  
SOURCE:

Dep. Chem., Saurashtra Univ., Rajkot, 360 005, India  
Journal of the Indian Chemical Society (1985), 62(3),  
255-7

CODEN: JICSAH; ISSN: 0019-4522

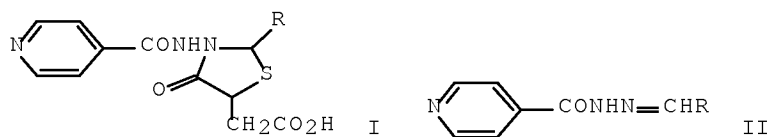
DOCUMENT TYPE:

Journal

LANGUAGE:

English

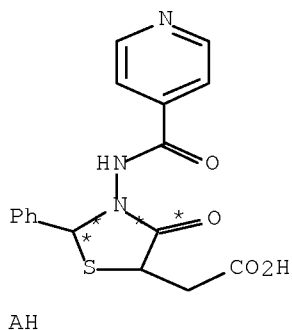
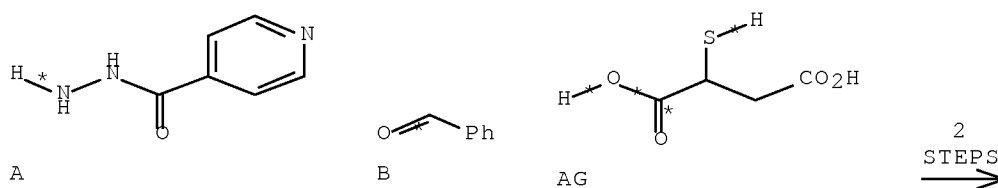
GI



AB     Fifteen thiazolidinones I [R = (un)substituted Ph, PhCH:CH, 2-furyl] were prepared by cyclization of the isoniazids II with thiomalic acid. Min. inhibitory concns. were determined for I and II against three bacteria.

RX(31) OF 45 COMPOSED OF RX(1), RX(16)

RX(31)     A + B + AG ==> AH



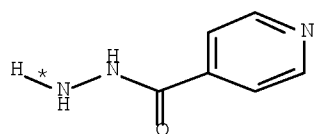
RX(1)     RCT    A 54-85-3, B 100-52-7

10/595943

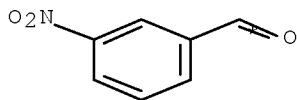
PRO C 533-02-8  
SOL 67-56-1 MeOH

RX(16) RCT C 533-02-8, AG 70-49-5  
RGT AI 7646-85-7 ZnCl2  
PRO AH 24327-74-0

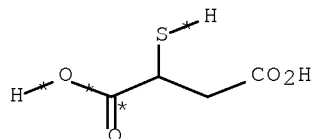
RX(32) OF 45 COMPOSED OF RX(2), RX(17)  
RX(32) A + E + AG ==> AJ



A

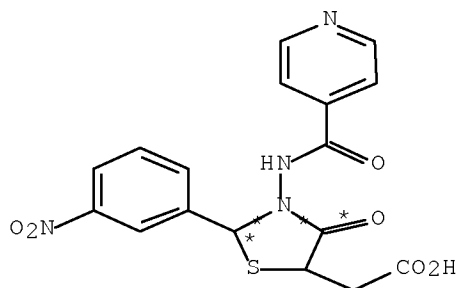


E



AG

2  
STEPS  
→



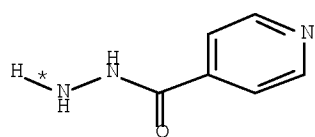
AJ

RX(2) RCT A 54-85-3, E 99-61-6  
PRO F 16012-26-3  
SOL 67-56-1 MeOH

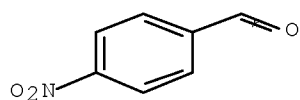
RX(17) RCT F 16012-26-3, AG 70-49-5  
RGT AI 7646-85-7 ZnCl2  
PRO AJ 103706-31-6

RX(33) OF 45 COMPOSED OF RX(3), RX(18)  
RX(33) A + G + AG ==> AK

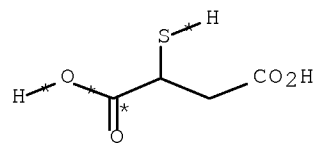
10/595943



A

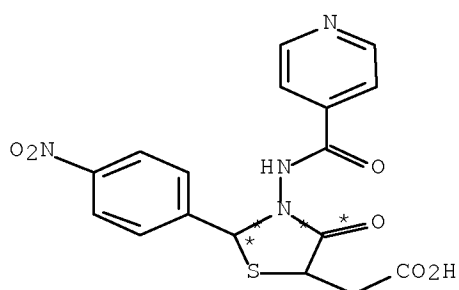


G



AG

2  
STEPS  
→

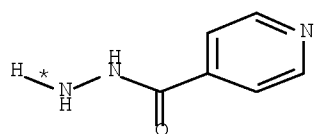


AK

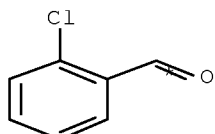
RX(3)      RCT    A 54-85-3, G 555-16-8  
              PRO    H 4813-07-4  
              SOL    67-56-1 MeOH

RX(18)     RCT    H 4813-07-4, AG 70-49-5  
              RGT    AI 7646-85-7 ZnCl2  
              PRO    AK 103706-32-7

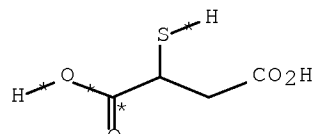
RX(34) OF 45 COMPOSED OF RX(4), RX(19)  
 RX(34)      A   +   I   +   AG   ==>   AL



A



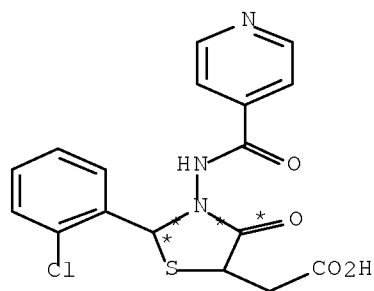
I



AG

10/595943

2  
STEPS  
→

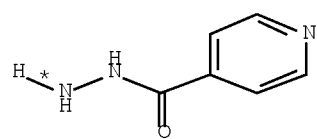


AL

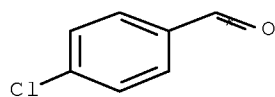
RX(4) RCT A 54-85-3, I 89-98-5  
PRO J 16012-25-2  
SOL 67-56-1 MeOH

RX(19) RCT J 16012-25-2, AG 70-49-5  
RGT AI 7646-85-7 ZnCl2  
PRO AL 36195-32-1

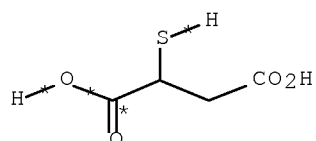
RX(35) OF 45 COMPOSED OF RX(5), RX(20)  
RX(35) A + K + AG ==> AM



A



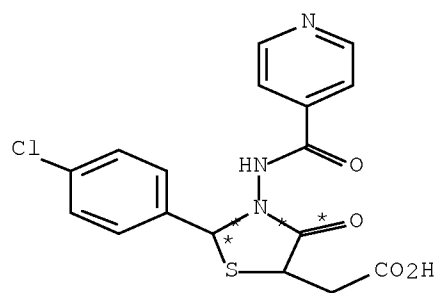
K



AG

2  
STEPS  
→

10/595943

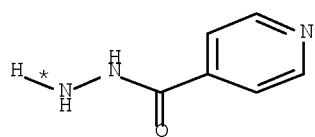


AM

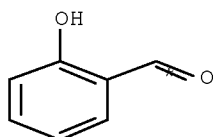
RX(5)      RCT    A 54-85-3, K 104-88-1  
              PRO    L 6342-46-7  
              SOL    67-56-1 MeOH

RX(20)     RCT    L 6342-46-7, AG 70-49-5  
              RGT    AI 7646-85-7 ZnCl2  
              PRO    AM 103710-50-5

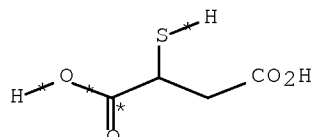
RX(36) OF 45 COMPOSED OF RX(6), RX(21)  
 RX(36)      A + M + AG ==> AN



A



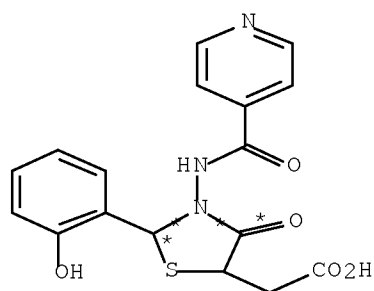
M



AG

2  
 STEPS  
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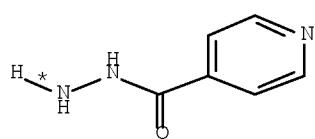


AN

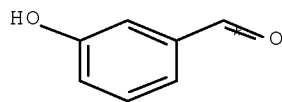
RX(6)        RCT    A 54-85-3, M 90-02-8  
               PRO    N 495-84-1  
               SOL    67-56-1 MeOH

RX(21)       RCT    N 495-84-1, AG 70-49-5  
               RGT    AI 7646-85-7 ZnCl2  
               PRO    AN 103706-33-8

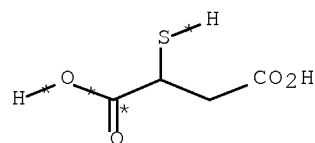
RX(37) OF 45 COMPOSED OF RX(7), RX(22)  
 RX(37)       A + O + AG ==> AG



A



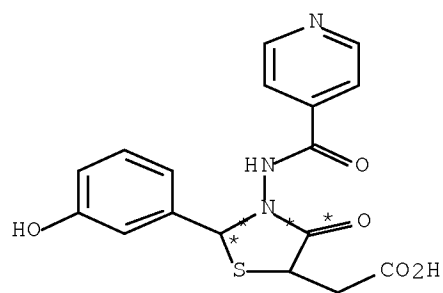
O



AG

2  
 STEPS  
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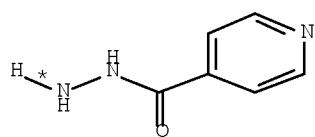


AO

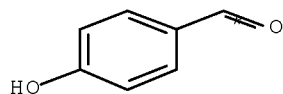
RX(7) RCT A 54-85-3, O 100-83-4  
 PRO P 840-80-2  
 SOL 67-56-1 MeOH

RX(22) RCT P 840-80-2, AG 70-49-5  
 RGT AI 7646-85-7 ZnCl2  
 PRO AO 103706-34-9

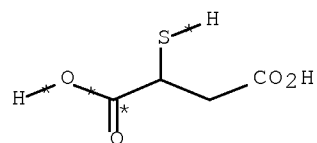
RX(38) OF 45 COMPOSED OF RX(8), RX(23)  
 RX(38) A + Q + AG ==> AP



A



Q

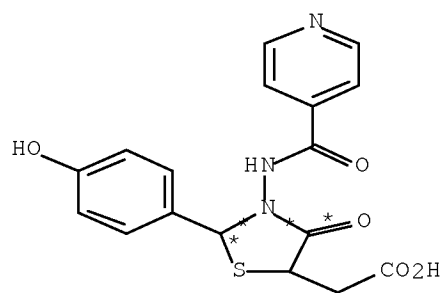


AG

2  
 STEPS  
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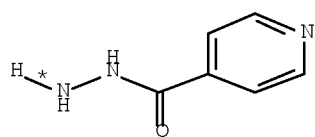


AP

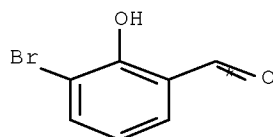
RX(8) RCT A 54-85-3, Q 123-08-0  
 PRO R 840-81-3  
 SOL 67-56-1 MeOH

RX(23) RCT R 840-81-3, AG 70-49-5  
 RGT AI 7646-85-7 ZnCl2  
 PRO AP 103706-35-0

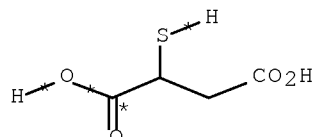
RX(39) OF 45 COMPOSED OF RX(9), RX(24)  
 RX(39) A + S + AG ==> AQ



A



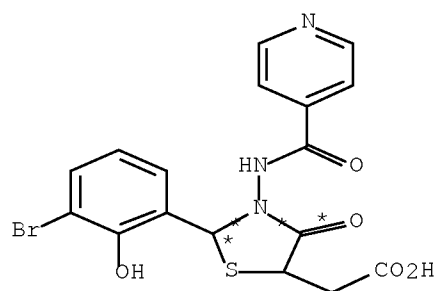
S



AG

2  
 STEPS  
 →

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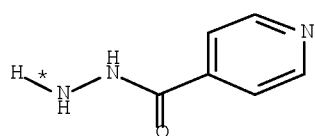


AQ

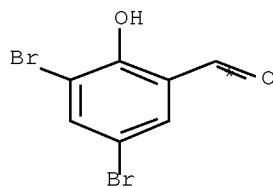
RX(9) RCT A 54-85-3, S 1829-34-1  
 PRO T 103706-30-5  
 SOL 67-56-1 MeOH

RX(24) RCT T 103706-30-5, AG 70-49-5  
 RGT AI 7646-85-7 ZnCl2  
 PRO AQ 103706-36-1

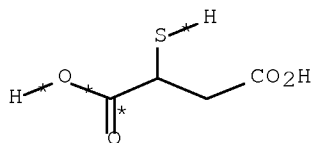
RX(40) OF 45 COMPOSED OF RX(10), RX(25)  
 RX(40) A + U + AG ==> AR



A



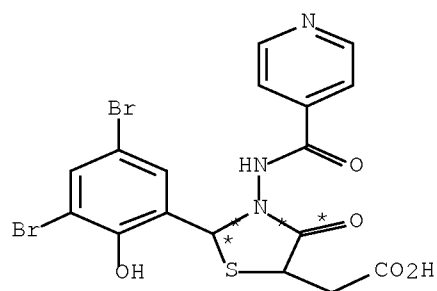
U



AG

2  
 STEPS  
 →

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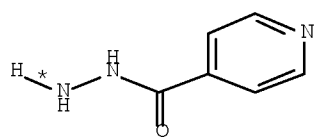


AR

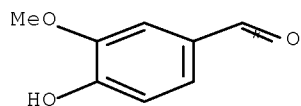
RX(10) RCT A 54-85-3, U 90-59-5  
 PRO V 68639-25-8  
 SOL 67-56-1 MeOH

RX(25) RCT V 68639-25-8, AG 70-49-5  
 RGT AI 7646-85-7 ZnCl2  
 PRO AR 103706-37-2

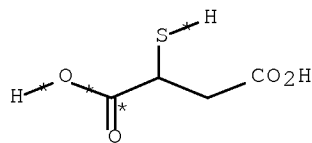
RX(41) OF 45 COMPOSED OF RX(11), RX(26)  
 RX(41) A + W + AG ==> AS



A



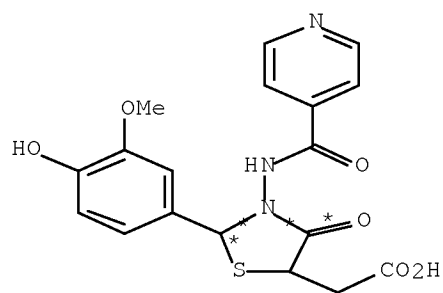
W



AG

2  
 STEPS  
 →

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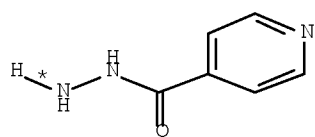


AS

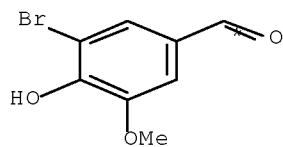
RX(11) RCT A 54-85-3, W 121-33-5  
 PRO X 149-17-7  
 SOL 67-56-1 MeOH

RX(26) RCT X 149-17-7, AG 70-49-5  
 RGT AI 7646-85-7 ZnCl2  
 PRO AS 103706-38-3

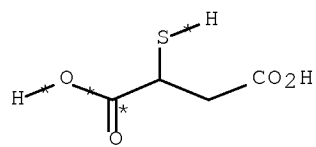
RX(42) OF 45 COMPOSED OF RX(12), RX(27)  
 RX(42) A + Y + AG ==> AT



A



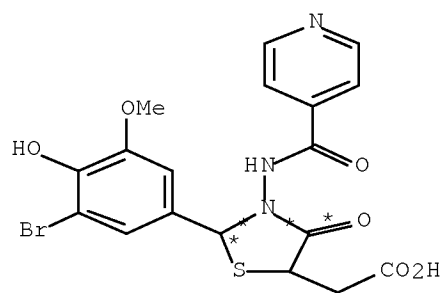
Y



AG

2  
 STEPS  
 →

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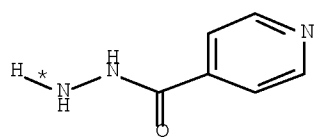


AT

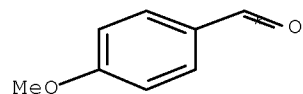
RX(12) RCT A 54-85-3, Y 2973-76-4  
 PRO Z 92160-05-9  
 SOL 67-56-1 MeOH

RX(27) RCT Z 92160-05-9, AG 70-49-5  
 RGT AI 7646-85-7 ZnCl2  
 PRO AT 103706-39-4

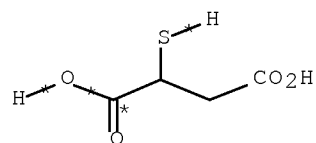
RX(43) OF 45 COMPOSED OF RX(13), RX(28)  
 RX(43) A + AA + AG ==> AU



A



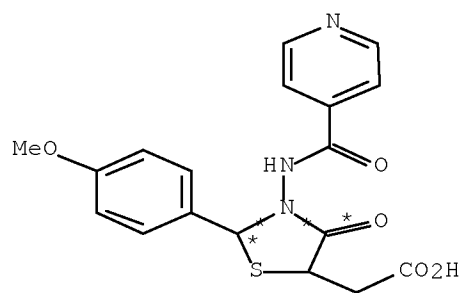
AA



AG

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 STEPS  
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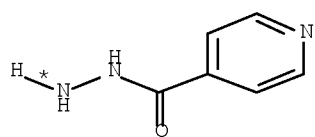


AU

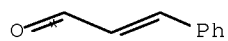
RX(13) RCT A 54-85-3, AA 123-11-5  
 PRO AB 893-42-5  
 SOL 67-56-1 MeOH

RX(28) RCT AB 893-42-5, AG 70-49-5  
 RGT AI 7646-85-7 ZnCl2  
 PRO AU 103706-40-7

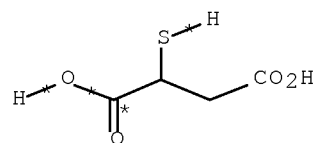
RX(44) OF 45 COMPOSED OF RX(14), RX(29)  
 RX(44) A + AC + AG ==> AV



A



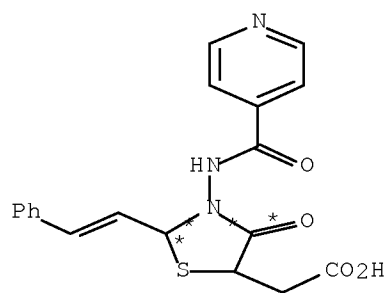
AC



AG

2  
 STEPS  
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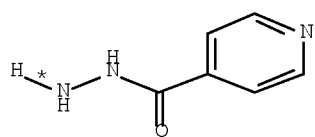


AV

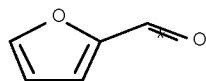
RX(14)      RCT    A 54-85-3, AC 104-55-2  
               PRO    AD 4813-11-0  
               SOL    67-56-1 MeOH

RX(29)      RCT    AD 4813-11-0, AG 70-49-5  
               RGT    AI 7646-85-7 ZnCl2  
               PRO    AV 103706-41-8

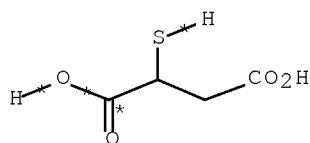
RX(45) OF 45 COMPOSED OF RX(15), RX(30)  
 RX(45)      A + AE + AG ==> AW



A



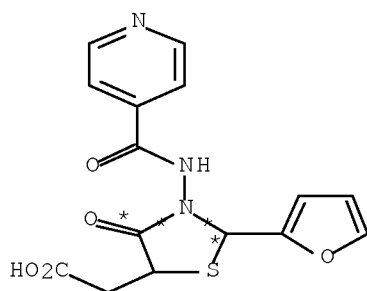
AE



AG

2  
 STEPS  
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AW

RX(15) RCT A 54-85-3, AE 98-01-1  
PRO AF 6956-53-2  
SOL 67-56-1 MeOH

RX(30) RCT AF 6956-53-2, AG 70-49-5  
RGT AI 7646-85-7 ZnCl2  
PRO AW 103706-42-9

L91 ANSWER 26 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 105:78864 CASREACT Full-text

TITLE: Studies on antitubercular agents. Preparation of  
1-(4-methoxybenzoyl)-2-benzalhydrazines and  
2-aryl-3-(4-methoxybenzamido)-5-carboxymethyl-4-  
thiazolidinones

AUTHOR(S): Patel, J. M.; Dave, M. P.; Langalia, N. A.; Thaker, K.  
A.

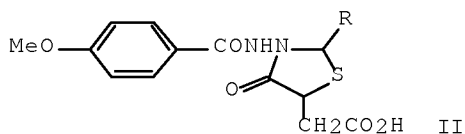
CORPORATE SOURCE: Dep. Chem., Bhavnagar Univ., Bhavnagar, 364 002, India  
SOURCE: Journal of the Indian Chemical Society (1985), 62(3),  
254-5

CODEN: JICSAH; ISSN: 0019-4522

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

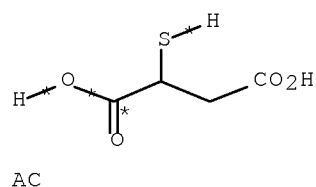
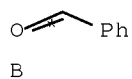
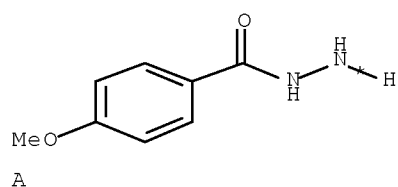


AB p-MeOC6H4CONHNH2 was condensed with RCHO [R = (un)substituted Ph, PhCH:CH] to give p-MeOC6H4CONHN:CHR (I) in 70-88% yield, which cyclized with HO2CCH2CH(SH)CO2H to give the thiazolidinones II in 55-76% yield. All I and II possess significant tuberculostatic activity at 30 µg/mL against Mycobacterium tuberculosis.

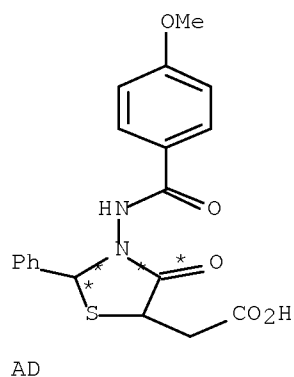


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RX(27) OF 39 COMPOSED OF RX(1), RX(14)  
 RX(27) A + B + AC ==> AD



2  
 STEPS  
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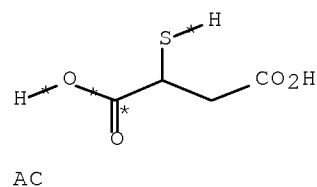
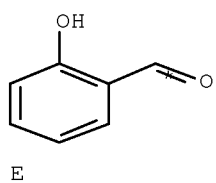
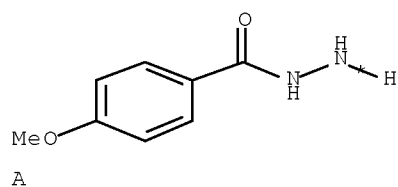


RX(1) RCT A 3290-99-1, B 100-52-7  
 PRO C 51651-81-1  
 SOL 64-17-5 EtOH

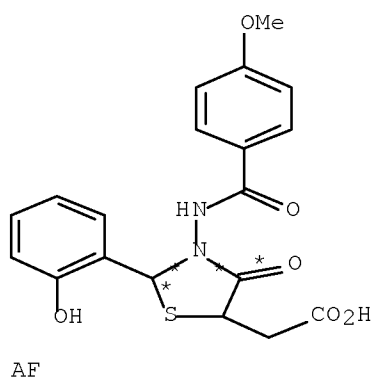
RX(14) RCT AC 70-49-5, C 51651-81-1  
 RGT AE 7646-85-7 ZnCl<sub>2</sub>  
 PRO AD 103635-31-0

RX(28) OF 39 COMPOSED OF RX(2), RX(15)  
 RX(28) A + E + AC ==> AF

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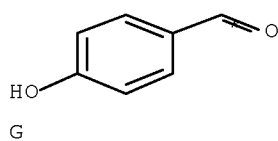
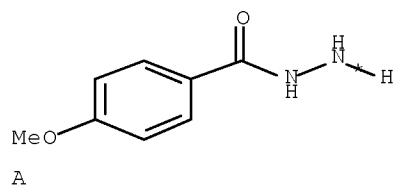
2  
STEPS  
→



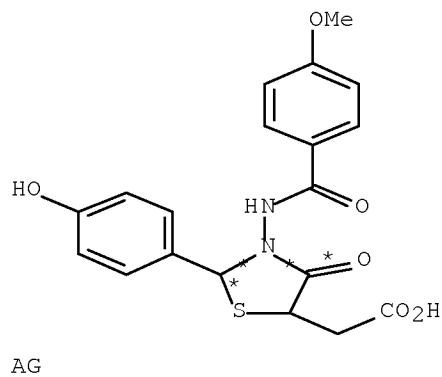
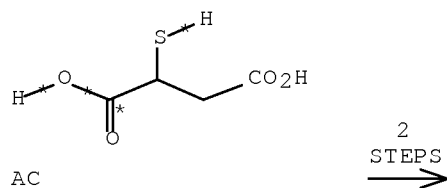
RX(2) RCT A 3290-99-1, E 90-02-8  
PRO F 100969-61-7  
SOL 64-17-5 EtOH

RX(15) RCT AC 70-49-5, F 100969-61-7  
RGT AE 7646-85-7 ZnCl2  
PRO AF 103635-32-1

RX(29) OF 39 COMPOSED OF RX(3), RX(16)  
RX(29) A + G + AC ==> AG



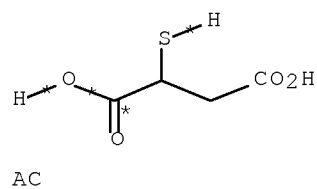
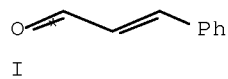
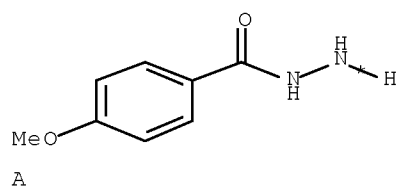
10/595943



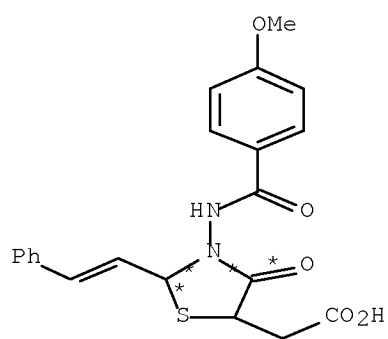
RX(3)      RCT    A 3290-99-1, G 123-08-0  
              PRO    H 103635-23-0  
              SOL    64-17-5 EtOH

RX(16)     RCT    AC 70-49-5, H 103635-23-0  
              RGT    AE 7646-85-7 ZnCl2  
              PRO    AG 103635-33-2

RX(30) OF 39 COMPOSED OF RX(4), RX(17)  
 RX(30)      A   +   I   +   AC   ==>   AH



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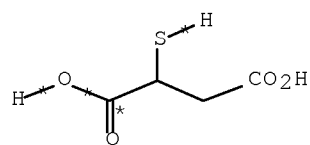
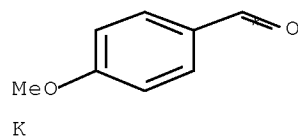
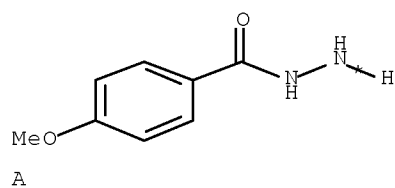
AH

RX(4)      RCT    A 3290-99-1, I 104-55-2  
              PRO    J 103635-24-1  
              SOL    64-17-5 EtOH

RX(17)     RCT    AC 70-49-5, J 103635-24-1  
              RGT    AE 7646-85-7 ZnCl2  
              PRO    AH 103635-34-3

RX(31) OF 39 COMPOSED OF RX(5), RX(18)

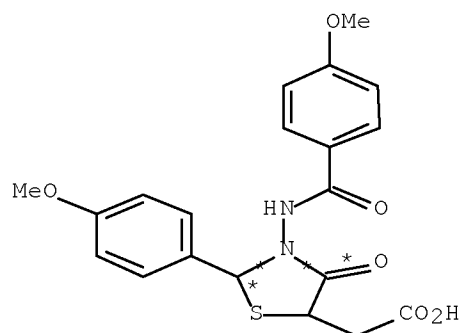
RX(31)      A + K + AC ==> AI



AC

2  
 STEPS  
 ➔

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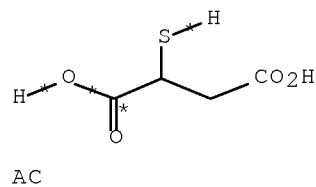
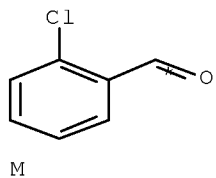
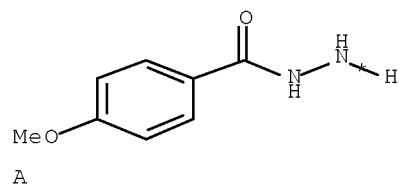


AI

RX(5) RCT A 3290-99-1, K 123-11-5  
 PRO L 51771-21-2  
 SOL 64-17-5 EtOH

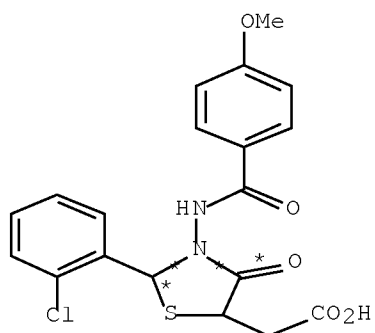
RX(18) RCT AC 70-49-5, L 51771-21-2  
 RGT AE 7646-85-7 ZnCl2  
 PRO AI 103635-35-4

RX(32) OF 39 COMPOSED OF RX(6), RX(19)  
 RX(32) A + M + AC ==> AJ



2  
 STEPS  
 →

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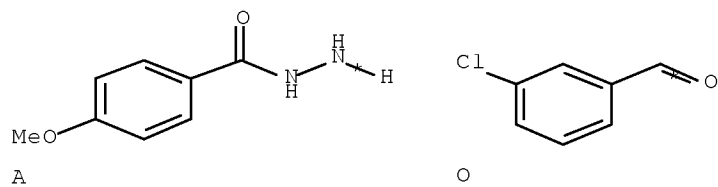


AJ

RX(6) RCT A 3290-99-1, M 89-98-5  
 PRO N 103635-25-2  
 SOL 64-17-5 EtOH

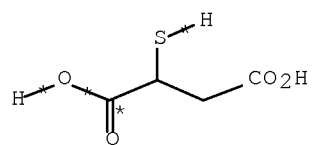
RX(19) RCT AC 70-49-5, N 103635-25-2  
 RGT AE 7646-85-7 ZnCl2  
 PRO AJ 103635-36-5

RX(33) OF 39 COMPOSED OF RX(7), RX(20)  
 RX(33) A + O + AC ==> AK



A

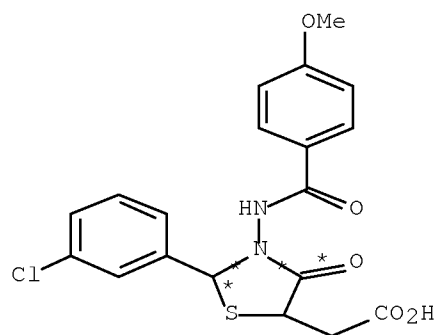
O



AC

2  
 STEPS  
 →

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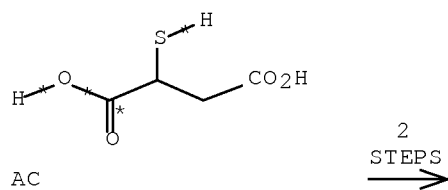
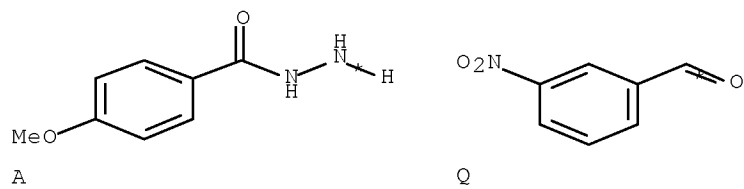
AK

RX(7) RCT A 3290-99-1, O 587-04-2  
 PRO P 103635-26-3  
 SOL 64-17-5 EtOH

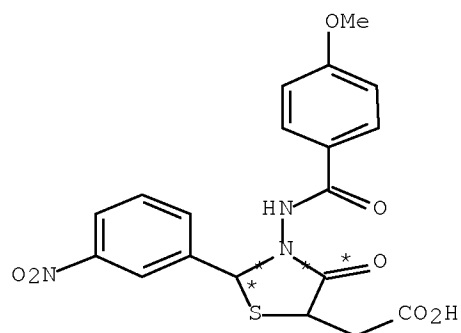
RX(20) RCT AC 70-49-5, P 103635-26-3  
 RGT AE 7646-85-7 ZnCl2  
 PRO AK 103635-37-6

RX(34) OF 39 COMPOSED OF RX(8), RX(21)

RX(34) A + Q + AC ==> AL



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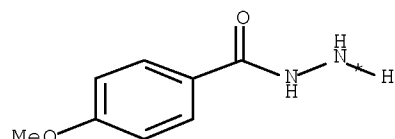


AL

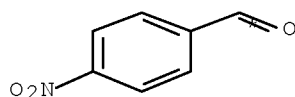
RX(8) RCT A 3290-99-1, Q 99-61-6  
 PRO R 103635-27-4  
 SOL 64-17-5 EtOH

RX(21) RCT AC 70-49-5, R 103635-27-4  
 RGT AE 7646-85-7 ZnCl2  
 PRO AL 103635-38-7

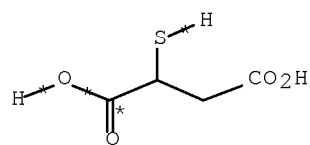
RX(35) OF 39 COMPOSED OF RX(9), RX(22)  
 RX(35) A + S + AC ==> AM



A



S

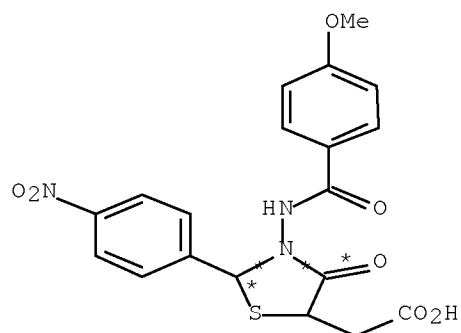


AC

2  
 STEPS  
 →



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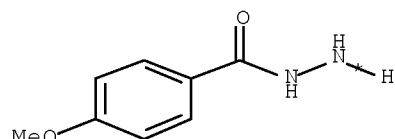


AM

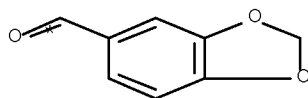
RX(9) RCT A 3290-99-1, S 555-16-8  
 PRO T 51771-23-4  
 SOL 64-17-5 EtOH

RX(22) RCT AC 70-49-5, T 51771-23-4  
 RGT AE 7646-85-7 ZnCl2  
 PRO AM 103635-39-8

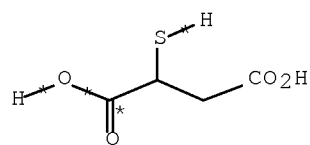
RX(36) OF 39 COMPOSED OF RX(10), RX(23)  
 RX(36) A + U + AC ==> AN



A



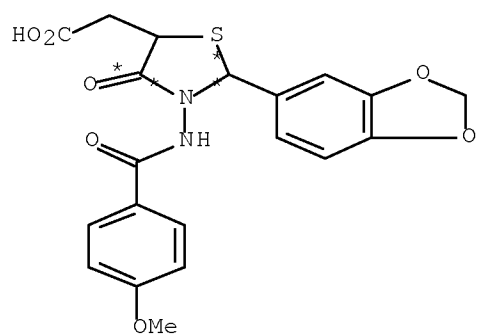
U



AC

2  
 STEPS  
 →

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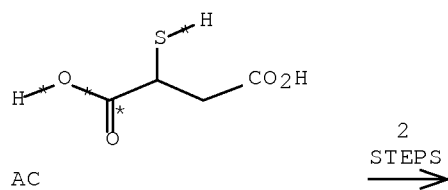
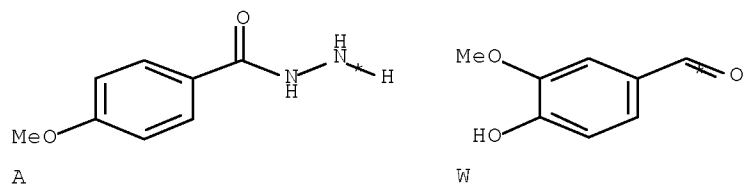


AN

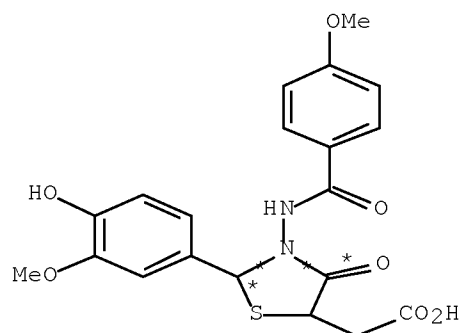
RX(10)      RCT    A 3290-99-1, U 120-57-0  
               PRO    V 103635-28-5  
               SOL    64-17-5 EtOH

RX(23)      RCT    AC 70-49-5, V 103635-28-5  
               RGT    AE 7646-85-7 ZnCl2  
               PRO    AN 103635-40-1

RX(37) OF 39 COMPOSED OF RX(11), RX(24)  
 RX(37)      A + W + AC ==> AO



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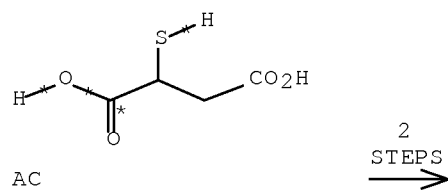
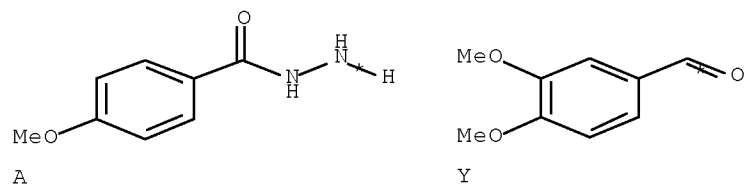


AO

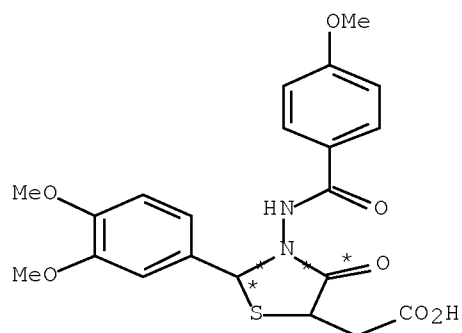
RX(11) RCT A 3290-99-1, W 121-33-5  
 PRO X 77218-64-5  
 SOL 64-17-5 EtOH

RX(24) RCT AC 70-49-5, X 77218-64-5  
 RGT AE 7646-85-7 ZnCl2  
 PRO AO 103635-41-2

RX(38) OF 39 COMPOSED OF RX(12), RX(25)  
 RX(38) A + Y + AC ==> AP



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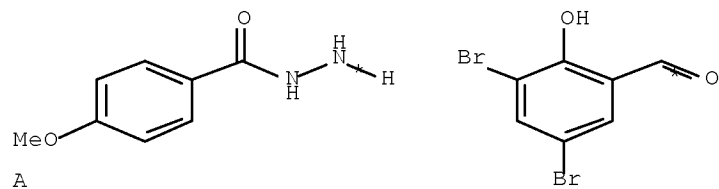


AP

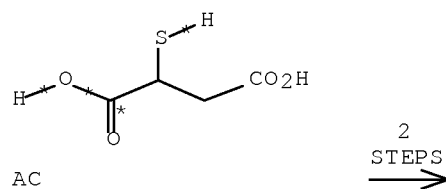
RX(12)      RCT    A 3290-99-1, Y 120-14-9  
               PRO    Z 103635-29-6  
               SOL    64-17-5 EtOH

RX(25)      RCT    AC 70-49-5, Z 103635-29-6  
              RGT    AE 7646-85-7 ZnCl2  
              PRO    AP 103635-42-3

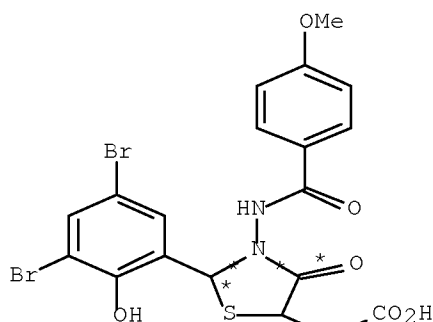
RX(39) OF 39 COMPOSED OF RX(13), RX(26)

$$\text{RX (39)} \quad \text{A} + \text{AA} + \text{AC} \implies \text{AQ}$$


AA



2  
STEPS  
→



AQ

RX(13) RCT A 3290-99-1, AA 90-59-5  
 PRO AB 103635-30-9  
 SOL 64-17-5 EtOH

RX(26) RCT AC 70-49-5, AB 103635-30-9  
 RGT AE 7646-85-7 ZnCl2  
 PRO AQ 103635-43-4

L91 ANSWER 27 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 104:207223 CASREACT Full-text

TITLE: Synthesis, saludiuretic, and antihypertensive activity  
 of 6,7-disubstituted 1(2H)- and  
 3,4-dihydro-1(2H)-phthalazinones

AUTHOR(S): Cherkez, S.; Herzig, J.; Yellin, H.

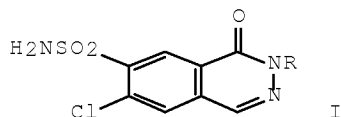
CORPORATE SOURCE: Teva Pharm. Ind. Ltd., Tel-Aviv, 61 013, Israel

SOURCE: Journal of Medicinal Chemistry (1986), 29(6), 947-59  
 CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



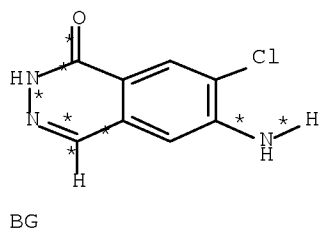
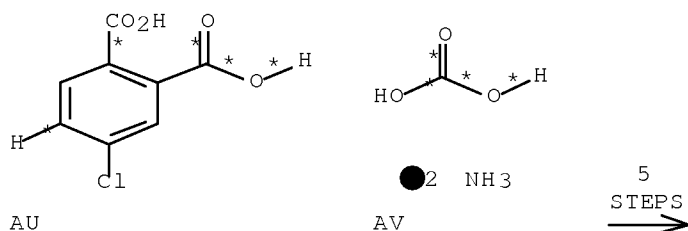
AB 6-Chloro-7-sulfamoyl-1(2H)-phthalazinones I (R = H, Me, PhCH<sub>2</sub>, m-CF<sub>3</sub>C<sub>6</sub>H<sub>4</sub>, furfuryl), four 7-chloro-6-sulfamoyl isomers (II), and their 3,4-dihydro derivs., combining structural features characteristic to furosemide and hydralazine, were prepared and their structure-activities relationships were studied. Preliminary screening in the rat shows that series I and dihydro derivs. exhibit diuretic and saluretic activity similar to that of chlorothiazide with, however, Na<sup>+</sup>/K<sup>+</sup> ratios more favorable than chlorothiazide and furosemide. The compds. of series II and dihydro derivs. are practically inactive. All four series show initial antihypertensive activity lower than that of hydralazine. However, I (R = H, PhCH<sub>2</sub>) and II (R = H) dihydro

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derivative show a higher activity at 8 and/or 24 h after administration and thus may offer a unique combination of a "loop" diuresis with direct long-acting peripheral vasodilating effects.

RX(149) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(28)

RX(149) AU + AV ==> BG



RX(23) RCT AU 89-20-3, AV 506-87-6  
PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2  
RGT BA 7697-37-2 HNO3  
PRO AZ 6015-57-2  
SOL 7664-93-9 H2SO4, 7732-18-5 Water

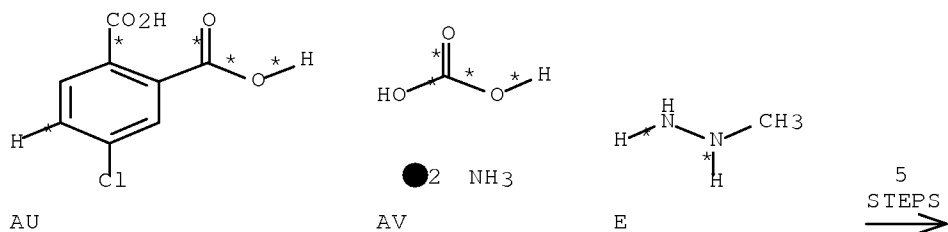
RX(26) RCT AZ 6015-57-2  
RGT BD 7772-99-8 SnCl2, M 7647-01-0 HCl  
PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3  
RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH  
PRO BE 100448-46-2  
SOL 7732-18-5 Water

RX(28) RCT BE 100448-46-2  
RGT C 302-01-2 N2H4  
PRO BG 100448-47-3  
SOL 7732-18-5 Water

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RX(150) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(29)  
 RX(150) AU + AV + E ==> BH



RX(23) RCT AU 89-20-3, AV 506-87-6  
 PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2  
 RGT BA 7697-37-2 HNO3  
 PRO AZ 6015-57-2  
 SOL 7664-93-9 H2SO4, 7732-18-5 Water

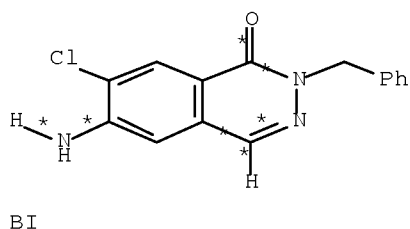
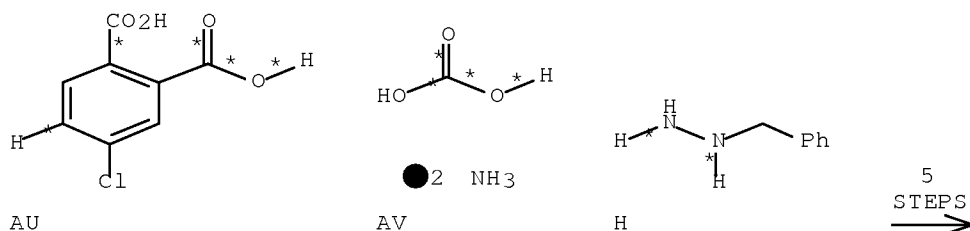
RX(26) RCT AZ 6015-57-2  
 RGT BD 7772-99-8 SnCl2, M 7647-01-0 HCl  
 PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3  
 RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt  
 (1:?), G 1310-73-2 NaOH  
 PRO BE 100448-46-2  
 SOL 7732-18-5 Water

RX(29) RCT BE 100448-46-2, E 60-34-4  
 PRO BH 100448-48-4  
 SOL 7732-18-5 Water

RX(151) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(30)  
 RX(151) AU + AV + H ==> BI

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RX(23) RCT AU 89-20-3, AV 506-87-6  
PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2  
RGT BA 7697-37-2 HNO3  
PRO AZ 6015-57-2  
SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2  
RGT BD 7772-99-8 SnCl2, M 7647-01-0 HCl  
PRO BC 5566-48-3

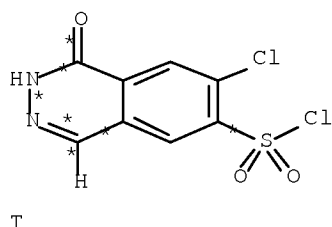
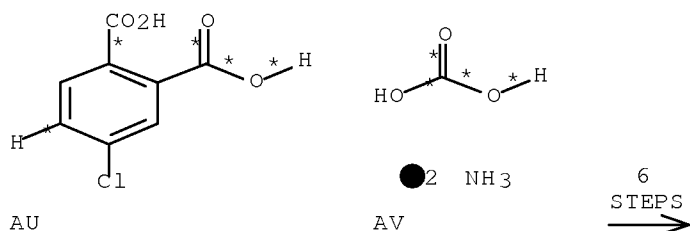
RX(27) RCT BC 5566-48-3  
RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH  
PRO BE 100448-46-2  
SOL 7732-18-5 Water

RX(30) RCT BE 100448-46-2, H 555-96-4  
PRO BI 100448-49-5  
SOL 7732-18-5 Water, 64-17-5 EtOH

RX(161) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(28), RX(32)  
RX(161) AU + AV ==> I



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RX(23) RCT AU 89-20-3, AV 506-87-6  
 PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2  
 RGT BA 7697-37-2 HNO<sub>3</sub>  
 PRO AZ 6015-57-2  
 SOL 7664-93-9 H<sub>2</sub>SO<sub>4</sub>, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2  
 RGT BD 7772-99-8 SnCl<sub>2</sub>, M 7647-01-0 HCl  
 PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3  
 RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH  
 PRO BE 100448-46-2  
 SOL 7732-18-5 Water

RX(28) RCT BE 100448-46-2  
 RGT C 302-01-2 N<sub>2</sub>H<sub>4</sub>  
 PRO BG 100448-47-3  
 SOL 7732-18-5 Water

RX(32) RCT BG 100448-47-3

STAGE(1)

RGT BM 7632-00-0 NaNO<sub>2</sub>  
 SOL 7732-18-5 Water

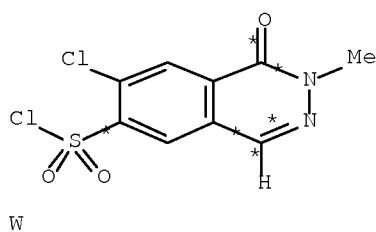
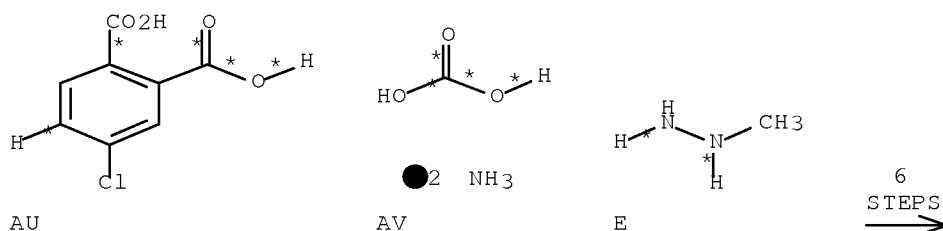
STAGE(2)

RGT BN 7758-89-6 CuCl, BO 7446-09-5 SO<sub>2</sub>  
 SOL 64-19-7 AcOH

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PRO T 100448-51-9

RX(162) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(29), RX(33)  
 RX(162) AU + AV + E ==> W



RX(23) RCT AU 89-20-3, AV 506-87-6  
 PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2  
 RGT BA 7697-37-2 HNO3  
 PRO AZ 6015-57-2  
 SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2  
 RGT BD 7772-99-8 SnCl2, M 7647-01-0 HCl  
 PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3  
 RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt  
 (1:?), G 1310-73-2 NaOH  
 PRO BE 100448-46-2  
 SOL 7732-18-5 Water

RX(29) RCT BE 100448-46-2, E 60-34-4  
 PRO BH 100448-48-4  
 SOL 7732-18-5 Water

RX(33) RCT BH 100448-48-4

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STAGE(1)

RGT BM 7632-00-0 NaNO<sub>2</sub>, M 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

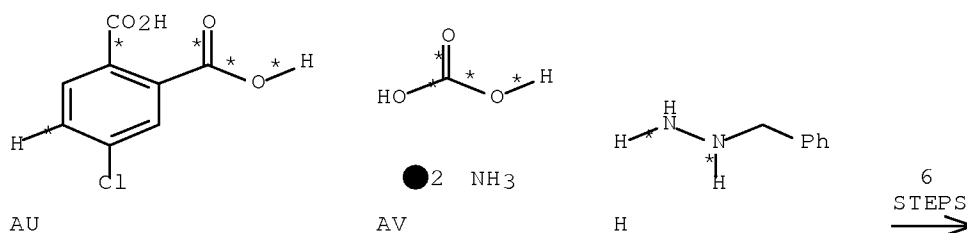
RGT BN 7758-89-6 CuCl, BO 7446-09-5 SO<sub>2</sub>

SOL 64-19-7 AcOH

PRO W 100448-52-0

RX(163) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(30), RX(34)

RX(163) AU + AV + H ==> Y



RX(23) RCT AU 89-20-3, AV 506-87-6  
PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2  
RGT BA 7697-37-2 HNO<sub>3</sub>  
PRO AZ 6015-57-2  
SOL 7664-93-9 H<sub>2</sub>SO<sub>4</sub>, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2  
RGT BD 7772-99-8 SnCl<sub>2</sub>, M 7647-01-0 HCl  
PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3  
RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH  
PRO BE 100448-46-2  
SOL 7732-18-5 Water

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RX(30) RCT BE 100448-46-2, H 555-96-4  
PRO BI 100448-49-5  
SOL 7732-18-5 Water, 64-17-5 EtOH

RX(34) RCT BI 100448-49-5

STAGE(1)

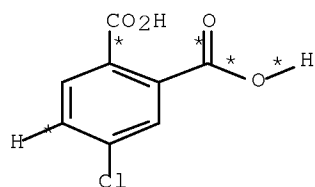
RGT BM 7632-00-0 NaNO<sub>2</sub>, M 7647-01-0 HCl  
SOL 7732-18-5 Water

STAGE(2)

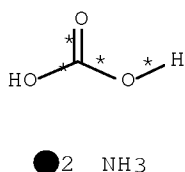
RGT BN 7758-89-6 CuCl, BO 7446-09-5 SO<sub>2</sub>  
SOL 64-19-7 AcOH

PRO Y 100448-53-1

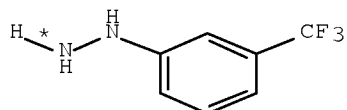
RX(164) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(39), RX(31)  
RX(164) AU + AV + BQ ==> BK



AU

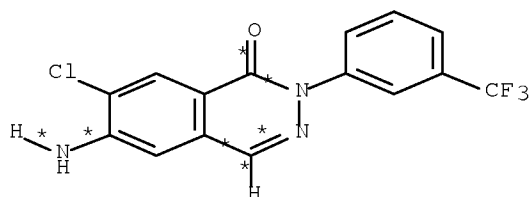


AV



BQ

6  
STEPS  
→



BK

RX(23) RCT AU 89-20-3, AV 506-87-6  
PRO AW 7147-90-2

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RX(25) RCT AW 7147-90-2  
 RGT BA 7697-37-2 HNO3  
 PRO AZ 6015-57-2  
 SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2  
 RGT BD 7772-99-8 SnCl2, M 7647-01-0 HCl  
 PRO BC 5566-48-3

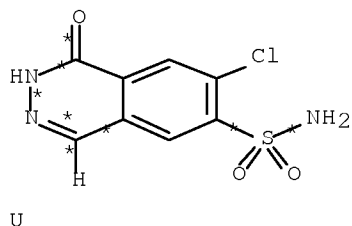
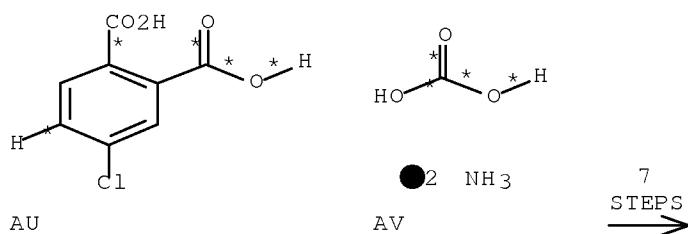
RX(27) RCT BC 5566-48-3  
 RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt  
 (1:?), G 1310-73-2 NaOH  
 PRO BE 100448-46-2  
 SOL 7732-18-5 Water

RX(39) RCT BE 100448-46-2, BQ 368-78-5  
 PRO BJ 100448-58-6  
 SOL 7732-18-5 Water, 64-17-5 EtOH

RX(31) RCT BJ 100448-58-6  
 PRO BK 100448-50-8  
 SOL 67-68-5 DMSO

RX(177) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(28), RX(32),  
 RX(7)

RX(177) AU + AV ==> U



RX(23) RCT AU 89-20-3, AV 506-87-6  
 PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2

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RGT BA 7697-37-2 HNO3  
 PRO AZ 6015-57-2  
 SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2  
 RGT BD 7772-99-8 SnCl2, M 7647-01-0 HCl  
 PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3  
 RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt  
 (1:?), G 1310-73-2 NaOH  
 PRO BE 100448-46-2  
 SOL 7732-18-5 Water

RX(28) RCT BE 100448-46-2  
 RGT C 302-01-2 N2H4  
 PRO BG 100448-47-3  
 SOL 7732-18-5 Water

RX(32) RCT BG 100448-47-3

STAGE(1)  
 RGT BM 7632-00-0 NaNO2  
 SOL 7732-18-5 Water

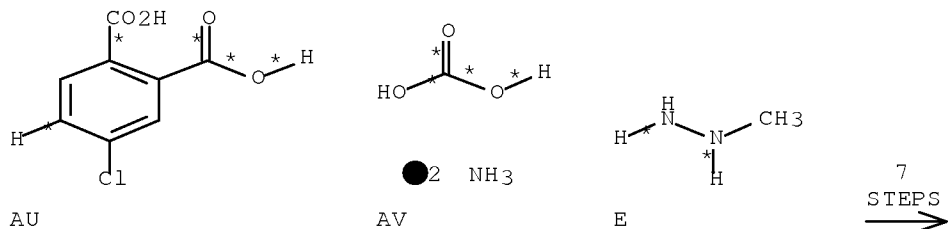
STAGE(2)  
 RGT BN 7758-89-6 CuCl, BO 7446-09-5 SO2  
 SOL 64-19-7 AcOH

PRO T 100448-51-9

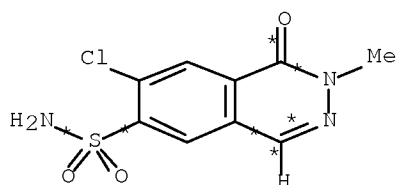
RX(7) RCT T 100448-51-9  
 RGT V 7664-41-7 NH3  
 PRO U 100448-31-5  
 SOL 7664-41-7 NH3

RX(178) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(29), RX(33),  
 RX(8)

RX(178) AU + AV + E ==> X



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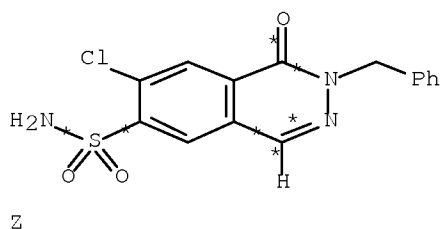
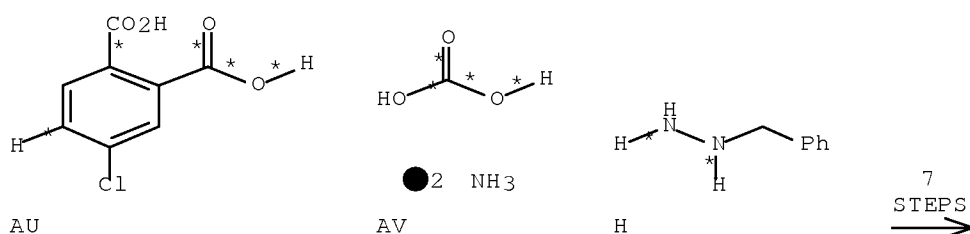


X

RX(23)	RCT	AU <del>89-20-3</del> , AV 506-87-6
	PRO	AW 7147-90-2
RX(25)	RCT	AW 7147-90-2
	RGT	BA 7697-37-2 HNO3
	PRO	AZ 6015-57-2
	SOL	7664-93-9 H2SO4, 7732-18-5 Water
RX(26)	RCT	AZ 6015-57-2
	RGT	BD <del>7772-99-8</del> SnCl2, M 7647-01-0 HCl
	PRO	BC 5566-48-3
RX(27)	RCT	BC 5566-48-3
	RGT	AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH
	PRO	BE 100448-46-2
	SOL	7732-18-5 Water
RX(29)	RCT	BE 100448-46-2, E <del>60-34-4</del>
	PRO	BH 100448-48-4
	SOL	7732-18-5 Water
RX(33)	RCT	BH 100448-48-4
	STAGE(1)	
	RGT	BM 7632-00-0 NaNO2, M 7647-01-0 HCl
	SOL	7732-18-5 Water
	STAGE(2)	
	RGT	BN <del>7758-89-6</del> CuCl, BO 7446-09-5 SO2
	SOL	64-19-7 AcOH
	PRO	W 100448-52-0
RX(8)	RCT	W 100448-52-0
	RGT	V 7664-41-7 NH3
	PRO	X <del>100448-32-6</del>
	SOL	7664-41-7 NH3

RX(179) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(30), RX(34),  
 RX(9)  
 RX(179) AU + AV + N ==> Z

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RX(23)	RCT	AU 89-20-3, AV 506-87-6
	PRO	AW 7147-90-2
RX(25)	RCT	AW 7147-90-2
	RGT	BA 7697-37-2 HNO3
	PRO	AZ 6015-57-2
	SOL	7664-93-9 H2SO4, 7732-18-5 Water
RX(26)	RCT	AZ 6015-57-2
	RGT	BD 7772-99-8 SnCl2, M 7647-01-0 HCl
	PRO	BC 5566-48-3
RX(27)	RCT	BC 5566-48-3
	RGT	AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH
	PRO	BE 100448-46-2
	SOL	7732-18-5 Water
RX(30)	RCT	BE 100448-46-2, H 555-96-4
	PRO	BI 100448-49-5
	SOL	7732-18-5 Water, 64-17-5 EtOH
RX(34)	RCT	BI 100448-49-5

STAGE(1)

RGT BM 7632-00-0 NaNO2, M 7647-01-0 HCl  
SOL 7732-18-5 Water

STAGE(2)

RGT BN 7758-89-6 CuCl, BO 7446-09-5 SO2  
SOL 64-19-7 AcOH

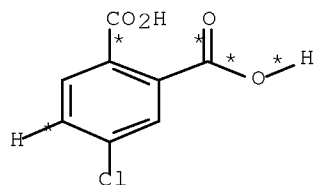


10/595943

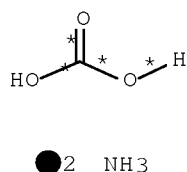
PRO Y 100448-53-1

RX(9) RCT Y 100448-53-1  
RGT V 7664-41-7 NH3  
PRO Z 100448-33-7  
SOL 7664-41-7 NH3

RX(180) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(39), RX(31),  
RX(35)  
RX(180) AU + AV + BQ ==> AA

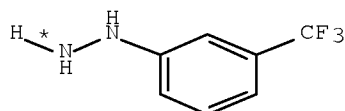


AU



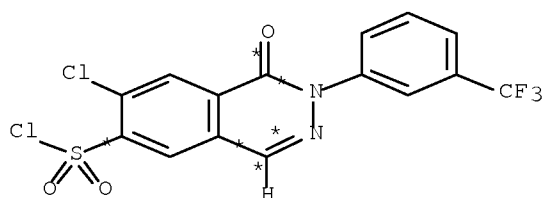
AV

●2 NH3



BQ

7  
STEPS  
→



AA

RX(23) RCT AU 89-20-3, AV 506-87-6  
PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2  
RGT BA 7697-37-2 HNO3  
PRO AZ 6015-57-2  
SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2  
RGT BD 7772-99-8 SnCl2, M 7647-01-0 HCl  
PRO BC 5566-48-3

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RX(27) RCT BC 5566-48-3  
RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt  
(1:?), G 1310-73-2 NaOH  
PRO BE 100448-46-2  
SOL 7732-18-5 Water

RX(39) RCT BE 100448-46-2, BQ 368-78-5  
PRO BJ 100448-58-6  
SOL 7732-18-5 Water, 64-17-5 EtOH

RX(31) RCT BJ 100448-58-6  
PRO BK 100448-50-8  
SOL 67-68-5 DMSO

RX(35) RCT BK 100448-50-8

STAGE(1)

RGT BM 7632-00-0 NaNO<sub>2</sub>, M 7647-01-0 HCl  
SOL 7732-18-5 Water

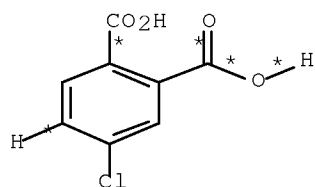
STAGE(2)

RGT BN 7758-89-6 CuCl, BO 7446-09-5 SO<sub>2</sub>  
SOL 64-19-7 AcOH

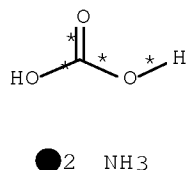
PRO AA 100448-54-2

RX(200) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(39), RX(31),  
RX(35), RX(10)

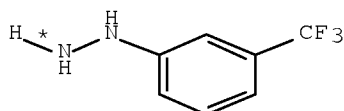
RX(200) AU + AV + BQ ==> AB



AU



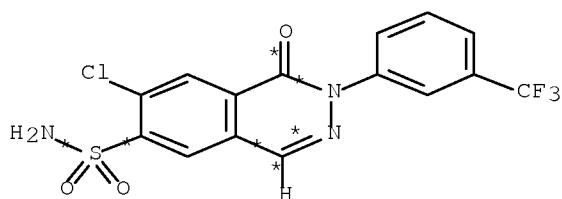
AV



BQ

8  
STEPS  
→

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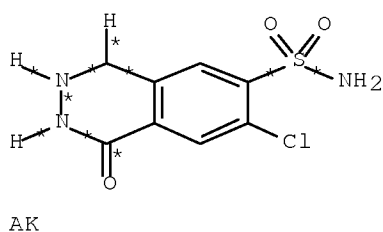
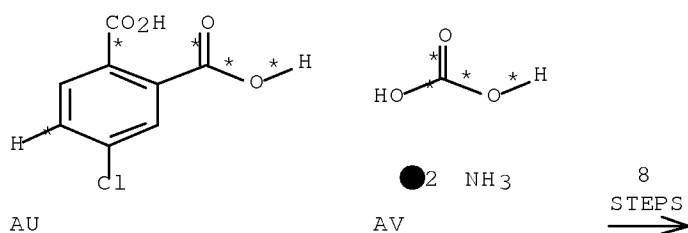
AB

RX(23)	RCT	AU <del>89-20-3</del> , AV 506-87-6
	PRO	AW 7147-90-2
RX(25)	RCT	AW 7147-90-2
	RGT	BA 7697-37-2 HNO3
	PRO	AZ 6015-57-2
	SOL	7664-93-9 H2SO4, 7732-18-5 Water
RX(26)	RCT	AZ 6015-57-2
	RGT	BD <del>7772-99-8</del> SnCl2, M 7647-01-0 HCl
	PRO	BC 5566-48-3
RX(27)	RCT	BC 5566-48-3
	RGT	AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH
	PRO	BE 100448-46-2
	SOL	7732-18-5 Water
RX(39)	RCT	BE 100448-46-2, BQ <del>368-78-5</del>
	PRO	BJ 100448-58-6
	SOL	7732-18-5 Water, 64-17-5 EtOH
RX(31)	RCT	BJ 100448-58-6
	PRO	BK 100448-50-8
	SOL	67-68-5 DMSO
RX(35)	RCT	BK 100448-50-8
	STAGE(1)	
	RGT	BM 7632-00-0 NaNO2, M 7647-01-0 HCl
	SOL	7732-18-5 Water
	STAGE(2)	
	RGT	BN <del>7758-89-6</del> CuCl, BO 7446-09-5 SO2
	SOL	64-19-7 AcOH
	PRO	AA 100448-54-2
RX(10)	RCT	AA 100448-54-2
	RGT	V 7664-41-7 NH3
	PRO	AB <del>100448-34-8</del>
	SOL	7664-41-7 NH3

RX(201) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(28), RX(32), RX(7), RX(17)

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RX(201) AU + AV ==> AK



RX(23) RCT AU 89-20-3, AV 506-87-6  
PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2  
RGT BA 7697-37-2 HNO3  
PRO AZ 6015-57-2  
SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2  
RGT BD 7772-99-8 SnCl2, M 7647-01-0 HCl  
PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3  
RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH  
PRO BE 100448-46-2  
SOL 7732-18-5 Water

RX(28) RCT BE 100448-46-2  
RGT C 302-01-2 N2H4  
PRO BG 100448-47-3  
SOL 7732-18-5 Water

RX(32) RCT BG 100448-47-3

STAGE(1)  
RGT BM 7632-00-0 NaNO2  
SOL 7732-18-5 Water

STAGE(2)

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RGT BN 7758-89-6 CuCl, BO 7446-09-5 SO2  
SOL 64-19-7 AcOH

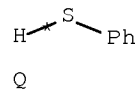
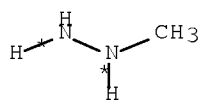
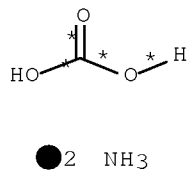
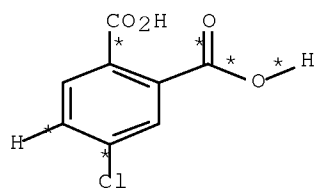
PRO T 100448-51-9

RX(7) RCT T 100448-51-9  
RGT V 7664-41-7 NH3  
PRO U 100448-31-5  
SOL 7664-41-7 NH3

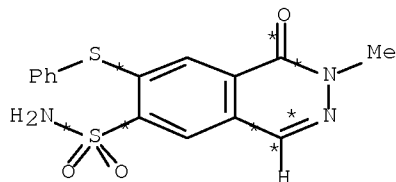
RX(17) RCT U 100448-31-5  
RGT AE 16940-66-2 NaBH4  
PRO AK 100448-41-7  
SOL 111-96-6 (MeOCH2CH2)2O

RX(202) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(29), RX(33),  
RX(8), RX(11)

RX(202) AU + AV + E + Q ==> AC



8  
STEPS  
→



RX(23) RCT AU 89-20-3, AV 506-87-6  
PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2  
RGT BA 7697-37-2 HNO3

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PRO AZ 6015-57-2  
SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2  
RGT BD ~~7772-99-8~~ SnCl2, M 7647-01-0 HCl  
PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3  
RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt  
(1:?), G 1310-73-2 NaOH  
PRO BE 100448-46-2  
SOL 7732-18-5 Water

RX(29) RCT BE 100448-46-2, E ~~60-34-4~~  
PRO BH 100448-48-4  
SOL 7732-18-5 Water

RX(33) RCT BH 100448-48-4

STAGE(1)

RGT BM 7632-00-0 NaNO2, M 7647-01-0 HCl  
SOL 7732-18-5 Water

STAGE(2)

RGT BN ~~7758-89-6~~ CuCl, BO 7446-09-5 SO2  
SOL 64-19-7 AcOH

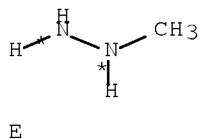
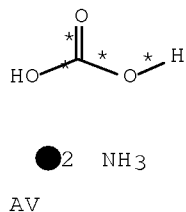
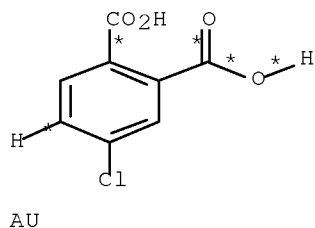
PRO W 100448-52-0

RX(8) RCT W 100448-52-0  
RGT V 7664-41-7 NH3  
PRO X 100448-32-6  
SOL 7664-41-7 NH3

RX(11) RCT X 100448-32-6, Q 108-98-5  
RGT S 144-55-8 NaHCO3  
PRO AC ~~100448-35-9~~  
SOL 7732-18-5 Water

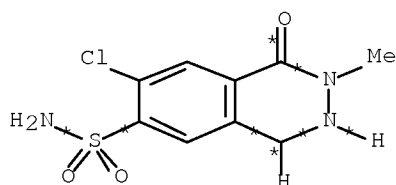
RX(203) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(29), RX(33),  
RX(8), RX(18)

RX(203) AU + AV + E ==> AL



8  
STEPS  
→

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AL

RX(23) RCT AU ~~89-20-3~~, AV 506-87-6  
PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2  
RGT BA 7697-37-2 HNO3  
PRO AZ 6015-57-2  
SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2  
RGT BD ~~7772-99-8~~ SnCl2, M 7647-01-0 HCl  
PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3  
RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt  
(1:?), G 1310-73-2 NaOH  
PRO BE 100448-46-2  
SOL 7732-18-5 Water

RX(29) RCT BE 100448-46-2, E ~~60-34-4~~  
PRO BH 100448-48-4  
SOL 7732-18-5 Water

RX(33) RCT BH 100448-48-4

STAGE(1)  
RGT BM 7632-00-0 NaNO2, M 7647-01-0 HCl  
SOL 7732-18-5 Water

STAGE(2)  
RGT BN ~~7758-89-6~~ CuCl, BO 7446-09-5 SO2  
SOL 64-19-7 AcOH

PRO W 100448-52-0

RX(8) RCT W 100448-52-0  
RGT V 7664-41-7 NH3  
PRO X 100448-32-6  
SOL 7664-41-7 NH3

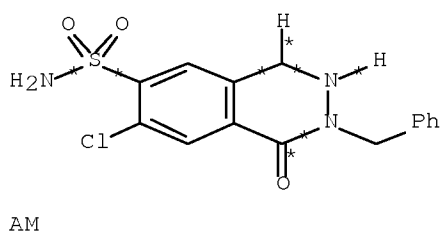
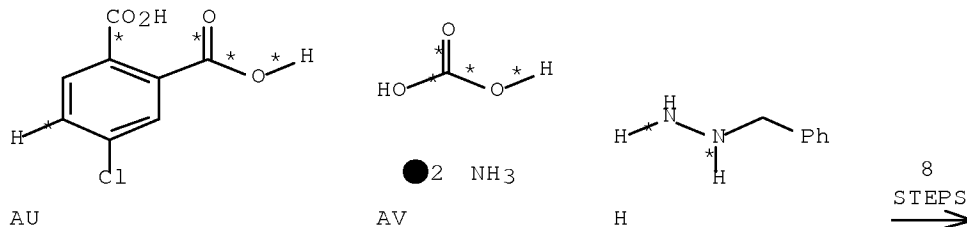
RX(18) RCT X 100448-32-6  
RGT AE 16940-66-2 NaBH4  
PRO AL ~~100448-42-8~~  
SOL 111-96-6 (MeOCH2CH2)2O

RX(204) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(30), RX(34),

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RX(9), RX(19)

RX(204) AU + AV + H ==> AM



RX(23) RCT AU 89-20-3, AV 506-87-6  
PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2  
RGT BA 7697-37-2 HNO3  
PRO AZ 6015-57-2  
SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2  
RGT BD 7772-99-8 SnCl2, M 7647-01-0 HCl  
PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3  
RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt  
(1:?), G 1310-73-2 NaOH  
PRO BE 100448-46-2  
SOL 7732-18-5 Water

RX(30) RCT BE 100448-46-2, H 555-96-4  
PRO BI 100448-49-5  
SOL 7732-18-5 Water, 64-17-5 EtOH

RX(34) RCT BI 100448-49-5

STAGE(1)

RGT BM 7632-00-0 NaNO2, M 7647-01-0 HCl  
SOL 7732-18-5 Water

STAGE(2)



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RGT BN 7758-89-6 CuCl, BO 7446-09-5 SO2  
SOL 64-19-7 AcOH

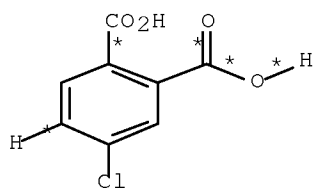
PRO Y 100448-53-1

RX(9) RCT Y 100448-53-1  
RGT V 7664-41-7 NH3  
PRO Z 100448-33-7  
SOL 7664-41-7 NH3

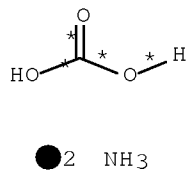
RX(19) RCT Z 100448-33-7  
RGT AE 16940-66-2 NaBH4  
PRO AM 100448-43-9  
SOL 111-96-6 (MeOCH2CH2)2O

RX(214) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(39), RX(31),  
RX(35), RX(10), RX(20)

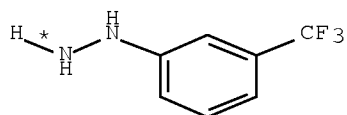
RX(214) AU + AV + BQ ==> AN



AU

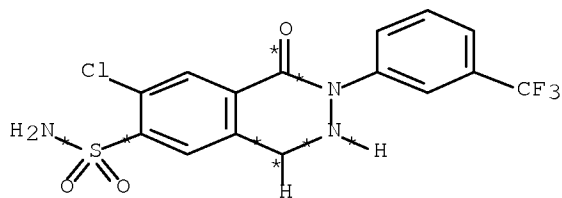


AV



BQ

9  
STEPS  
→



AN

RX(23) RCT AU 89-20-3, AV 506-87-6  
PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2  
RGT BA 7697-37-2 HNO3

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PRO AZ 6015-57-2  
SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2  
RGT BD ~~7772-99-8~~ SnCl2, M 7647-01-0 HCl  
PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3  
RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt  
(1:?), G 1310-73-2 NaOH  
PRO BE 100448-46-2  
SOL 7732-18-5 Water

RX(39) RCT BE 100448-46-2, BQ ~~368-78-5~~  
PRO BJ 100448-58-6  
SOL 7732-18-5 Water, 64-17-5 EtOH

RX(31) RCT BJ 100448-58-6  
PRO BK 100448-50-8  
SOL 67-68-5 DMSO

RX(35) RCT BK 100448-50-8

STAGE(1)  
RGT BM 7632-00-0 NaNO2, M 7647-01-0 HCl  
SOL 7732-18-5 Water

STAGE(2)  
RGT BN ~~7758-89-6~~ CuCl, BO 7446-09-5 SO2  
SOL 64-19-7 AcOH

PRO AA 100448-54-2

RX(10) RCT AA 100448-54-2  
RGT V 7664-41-7 NH3  
PRO AB 100448-34-8  
SOL 7664-41-7 NH3

RX(20) RCT AB 100448-34-8  
RGT AE 16940-66-2 NaBH4  
PRO AN ~~100448-44-0~~  
SOL 111-96-6 (MeOCH2CH2)2O

L91 ANSWER 28 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 104:129829 CASREACT Full-text

TITLE: Synthesis and antitubercular activity of some  
2-aryl-3-(4-chlorobenzamido)-5-substituted-4-  
thiazolidinones

AUTHOR(S): Dave, M. P.; Patel, J. M.; Langalia, N. A.; Thaker, K.  
A.

CORPORATE SOURCE: Dep. Chem., Bhavnagar Univ., Bhavnagar, 364 002, India  
SOURCE: Journal of the Indian Chemical Society (1984), 61(10),  
891-2

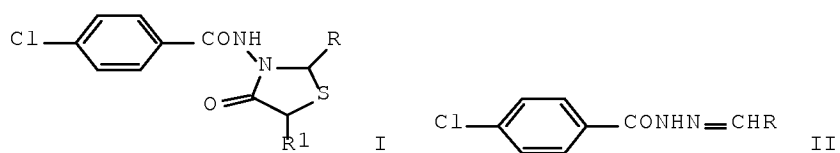
CODEN: JICSAH; ISSN: 0019-4522

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

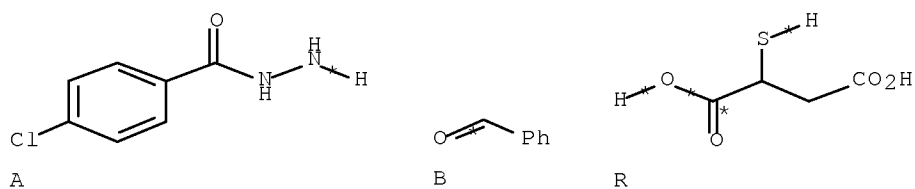
10/595943



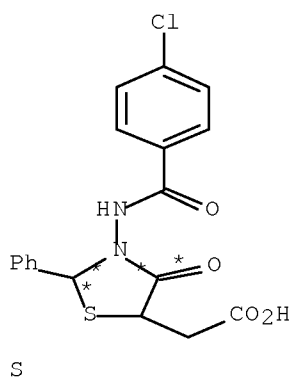
AB Title compds. I (R = Ph, C<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>-2, C<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>-4, C<sub>6</sub>H<sub>4</sub>OMe-4, C<sub>6</sub>H<sub>3</sub>(OMe)<sub>2</sub>-3,4; R<sub>1</sub> = H, Me, CH<sub>2</sub>CO<sub>2</sub>H) were prepared by condensation of Schiff bases II with mercaptoalkanoic acids. I show antitubercular activity against Hs7Rv strain at 30 µg/mL in vitro.

RX(21) OF 33 COMPOSED OF RX(1), RX(8)

RX(21) A + B + R ==> S



2  
STEPS  
→



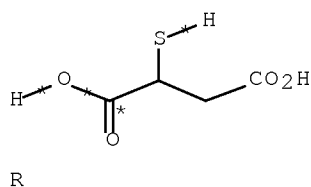
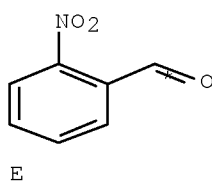
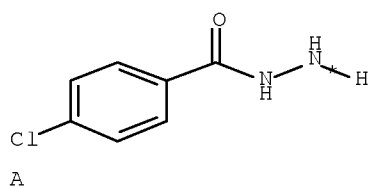
RX(1) RCT A 536-40-3, B 100-52-7

10/595943

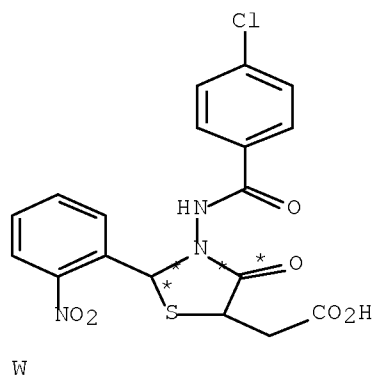
PRO C 31061-81-1  
SOL 64-17-5 EtOH

RX(8) RCT R 70-49-5, C 31061-81-1  
RGT T 7646-85-7 ZnCl2  
PRO S 101125-20-6

RX(24) OF 33 COMPOSED OF RX(2), RX(11)  
RX(24) A + E + R ==> W



2  
STEPS  
→

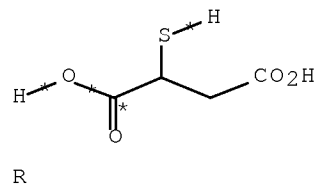
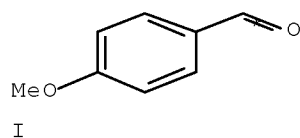
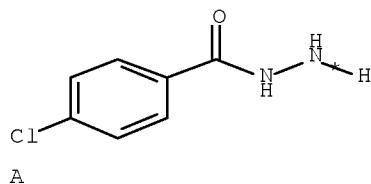


RX(2) RCT A 536-40-3, E 552-89-6  
PRO F 62982-45-0  
SOL 64-17-5 EtOH

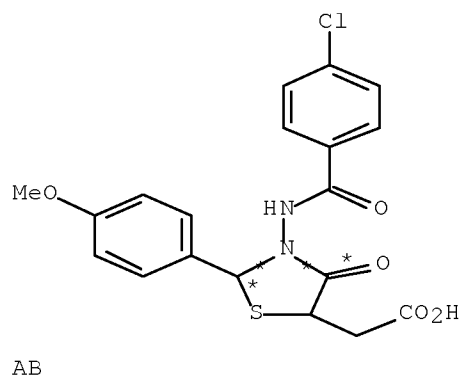
RX(11) RCT R 70-49-5, F 62982-45-0  
RGT T 7646-85-7 ZnCl2  
PRO W 101125-21-7

RX(30) OF 33 COMPOSED OF RX(4), RX(16)  
RX(30) A + I + R ==> AE

10/595943



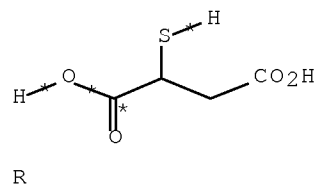
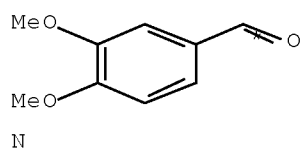
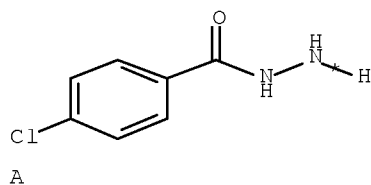
2  
STEPS  
→



RX(4) RCT A 536-40-3, I 123-11-5  
PRO J 51771-28-9  
SOL 64-17-5 EtOH

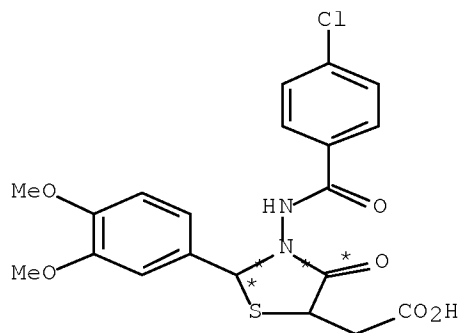
RX(16) RCT R 70-49-5, J 51771-28-9  
RGT T 7646-85-7 ZnCl2  
PRO AB 101125-23-9

RX(32) OF 33 COMPOSED OF RX(6), RX(18)  
RX(32) A + N + R ==> AD



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2  
STEPS  
→



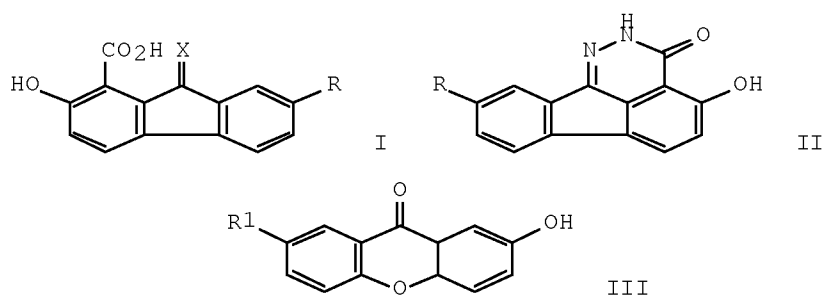
AD

RX(6) RCT A 536-40-3, N 120-14-9  
PRO O 101125-30-8  
SOL 64-17-5 EtOH

RX(18) RCT R 70-49-5, O 101125-30-8  
RGT T 7646-85-7 ZnCl2  
PRO AD 101125-24-0

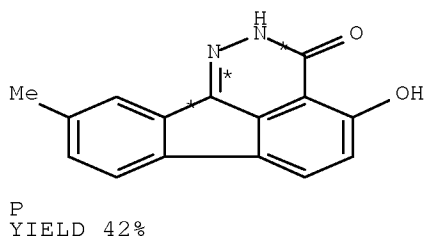
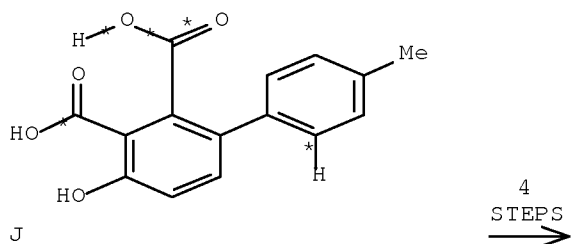
L91 ANSWER 29 OF 30 CASREACT COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 100:139054 CASREACT [Full-text](#)  
TITLE: 3-Aryl- and 3-(aryloxy)phthalic acids in the synthesis  
of fluorenones and xanthenes  
AUTHOR(S): Oleinik, A. F.; Adamskaya, E. V.  
CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow,  
119021, USSR  
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1983), (11),  
1537-9  
CODEN: KGSSAQ; ISSN: 0453-8234  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian  
GI

10/595943



AB    Fluorenones I (R = Me, OH, X = O), prepared in 70 and 66% from the corresponding phthalic anhydride, were treated with N<sub>2</sub>H<sub>4</sub>.H<sub>2</sub>O to give 76% I (X = NNH<sub>2</sub>), which underwent intramol. cyclocondensation by heating in vacuo at 180-200° to give 42% II. Xanthenones III (R<sub>1</sub> = Me, H) were also obtained from the corresponding 3-phenoxyphthalic anhydride.

RX(32) OF 36 COMPOSED OF RX(4), RX(6), RX(1), RX(9)  
 RX(32)    J    ==>    P



RX(4)        RCT    J 84185-83-1  
               PRO    K 84207-12-5

RX(6)        RCT    K 84207-12-5

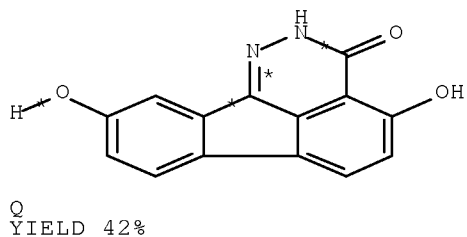
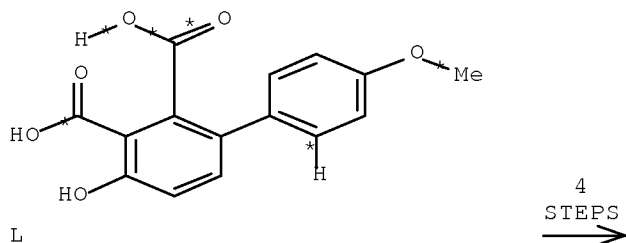
10/595943

RGT N 7446-70-0 AlCl3  
PRO A 89450-81-7

RX(1) RCT A 89450-81-7  
RGT C 302-01-2 N2H4, D 7732-18-5 Water  
PRO B 89450-83-9  
SOL 7732-18-5 Water

RX(9) RCT B 89450-83-9  
PRO P 89450-85-1

RX(34) OF 36 COMPOSED OF RX(5), RX(7), RX(8), RX(10)  
RX(34) L ==> Q



RX(5) RCT L 84185-84-2  
PRO M 84185-72-8

RX(7) RCT M 84185-72-8  
RGT N 7446-70-0 AlCl3  
PRO G 89450-82-8

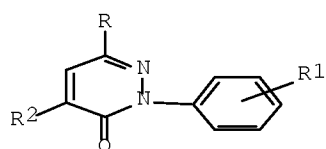
RX(8) RCT G 89450-82-8  
RGT C 302-01-2 N2H4, D 7732-18-5 Water  
PRO O 89450-84-0  
SOL 7732-18-5 Water

RX(10) RCT O 89450-84-0  
PRO Q 89450-86-2



10/595943

ACCESSION NUMBER: 93:46557 CASREACT Full-text  
 TITLE: Synthesis of the derivatives of  
 1-methoxyphenyl-3-hydroxypyridazin-6-ones. I.  
 Chlorination and substitution reactions  
 AUTHOR(S): Baloniak, Sylwester; Linkowska, Ewa;  
 Zyczynska-Baloniak, Irena  
 CORPORATE SOURCE: Inst. Chem. Anal., Sch. Med., Poznan, Pol.  
 SOURCE: Acta Poloniae Pharmaceutica (1979), 36(3), 301-6  
 CODEN: APPHAX; ISSN: 0001-6837  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Polish  
 GI

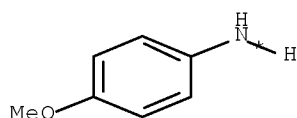


I, R=OH, R2=H, R1 as in text  
 II, R=Cl, R2=H, R1 as in text  
 III, R=R2=Cl, R1 as in text  
 IV, R=Cl, R1 and R2 as in text

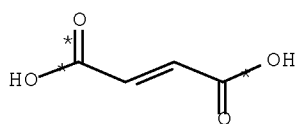
AB 3- And 4-MeOC6H4NHNH2-HCl refluxed with maleic anhydride in AcOH-AcONa gave I (R1 = 3- and 4-MeO, resp.). In preparation of I (R1 = 2-MeO), the intermediate 2-MeOC6H4NHNHCOCH:CHCO2H was isolated and cyclized with HCl. I were converted into the corresponding II by reaction with POCl3, whereas heating I in PCl5-POCl3 gave III. III heated with amines in DMF or alcs. gave 7 new IV (R2 = NHNH2, NEt2, 4-morpholinyl); IV (R2 = OMe) was obtained as the main product in the reaction of III with Et2NH.

RX(47) OF 66 COMPOSED OF RX(1), RX(2), RX(10), RX(16)

RX(47) A + E ==> AE



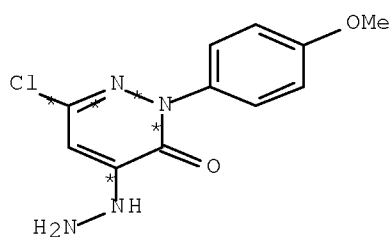
A



E

4  
STEPS  
→

10/595943



AB  
YIELD 71%

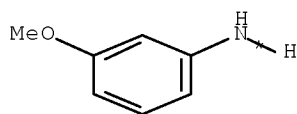
RX(1) RCT A 104-94-9  
RGT C 7782-77-6 HNO<sub>2</sub>, D 7772-99-8 SnCl<sub>2</sub>  
PRO B 19501-58-7

RX(2) RCT B 19501-58-7, E 6915-18-0  
RGT G 7647-01-0 HCl  
PRO F 60399-10-2

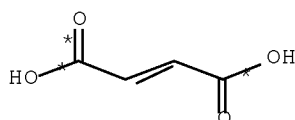
RX(10) RCT F 60399-10-2  
RGT N 10025-87-3 POCl<sub>3</sub>, R 10026-13-8 PCl<sub>5</sub>  
PRO S 73924-41-1

RX(16) RCT S 73924-41-1  
RGT X 302-01-2 N<sub>2</sub>H<sub>4</sub>  
PRO AB 73924-47-7

RX(61) OF 66 COMPOSED OF RX(20), RX(5), RX(9), RX(14)  
RX(61) AH + E ==> Z

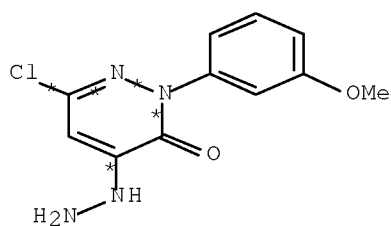


AH



E

4  
STEPS  
→



Z  
YIELD 51%

10/595943

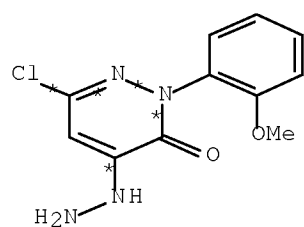
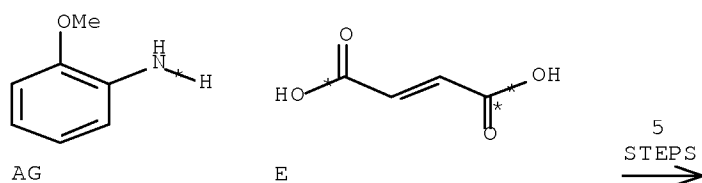
RX(20) RCT AH 536-90-3  
RGT C 7782-77-6 HNO2, D 7772-99-8 SnCl2  
PRO K 39232-91-2

RX(5) RCT K 39232-91-2, E 6915-18-0  
RGT G 7647-01-0 HCl  
PRO L 73924-35-3

RX(9) RCT L 73924-35-3  
RGT N 10025-87-3 POC13, R 10026-13-8 PC15  
PRO Q 73924-40-0

RX(14) RCT Q 73924-40-0  
RGT X 302-01-2 N2H4  
PRO Z 73924-46-6

RX(66) OF 66 COMPOSED OF RX(19), RX(3), RX(4), RX(21), RX(12)  
RX(66) AG + E ==> W



W  
YIELD 51%

RX(19) RCT AG 90-04-0  
RGT C 7782-77-6 HNO2, D 7772-99-8 SnCl2  
PRO H 6971-45-5

RX(3) RCT H 6971-45-5, E 6915-18-0  
PRO I 344876-90-0

RX(4) RCT I 344876-90-0

10/595943

RGT G 7647-01-0 HCl  
PRO J 60399-12-4

RX(21) RCT J 60399-12-4  
RGT N 10025-87-3 POC13, R 10026-13-8 PC15  
PRO T 73924-39-7

RX(12) RCT T 73924-39-7  
RGT X 302-01-2 N2H4  
PRO W 73924-45-5

10/595943

=> d his full

(FILE 'HOME' ENTERED AT 08:10:30 ON 17 OCT 2008)

FILE 'REGISTRY' ENTERED AT 08:15:23 ON 17 OCT 2008

ACT JAI943APPRNS/A

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L1           38 SEA ABB=ON PLU=ON (10025-73-7/BI OR 10025-91-9/BI OR  
              10026-07-0/BI OR 10026-10-5/BI OR 10026-11-6/BI OR 10026-12-7/B  
              I OR 10049-06-6/BI OR 10108-64-2/BI OR 10294-34-5/BI OR  
              123-91-1/BI OR 13450-90-3/BI OR 22441-45-8/BI OR 3682-15-3/BI  
              OR 521-31-3/BI OR 603-11-2/BI OR 67-64-1/BI OR 67-68-5/BI OR  
              68-12-2/BI OR 7446-70-0/BI OR 7447-39-4/BI OR 7487-94-7/BI OR  
              7550-45-0/BI OR 7637-07-2/BI OR 7646-79-9/BI OR 7646-85-7/BI  
              OR 7647-18-9/BI OR 7697-37-2/BI OR 7705-07-9/BI OR 7705-08-0/BI  
              OR 7718-54-9/BI OR 7758-89-6/BI OR 7784-34-1/BI OR 7786-30-3/B  
              I OR 7787-47-5/BI OR 7787-60-2/BI OR 7789-48-2/BI OR 85-44-9/BI  
              OR 872-50-4/BI)

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ACT JAI943CATRNS/A

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L2           28 SEA ABB=ON PLU=ON (10025-73-7/BI OR 10025-91-9/BI OR  
              10026-07-0/BI OR 10026-10-5/BI OR 10026-11-6/BI OR 10026-12-7/B  
              I OR 10049-06-6/BI OR 10108-64-2/BI OR 10294-34-5/BI OR  
              13450-90-3/BI OR 22441-45-8/BI OR 7446-70-0/BI OR 7447-39-4/BI  
              OR 7487-94-7/BI OR 7550-45-0/BI OR 7637-07-2/BI OR 7646-79-9/BI  
              OR 7646-85-7/BI OR 7647-18-9/BI OR 7705-07-9/BI OR 7705-08-0/B  
              I OR 7718-54-9/BI OR 7758-89-6/BI OR 7784-34-1/BI OR 7786-30-3/  
              BI OR 7787-47-5/BI OR 7787-60-2/BI OR 7789-48-2/BI)

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ACT JAI943SOLRNS/A

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L3           5 SEA ABB=ON PLU=ON (123-91-1/BI OR 67-64-1/BI OR 67-68-5/BI  
              OR 68-12-2/BI OR 872-50-4/BI)

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L4           5 SEA ABB=ON PLU=ON L1 NOT (L2 OR L3)  
              D SCA

FILE 'ZCAPLUS' ENTERED AT 08:17:38 ON 17 OCT 2008

ACT JAI943APP/A

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L5           1 SEA ABB=ON PLU=ON US2006-595943/AP  
              D SCA

FILE 'CASREACT' ENTERED AT 08:22:57 ON 17 OCT 2008

L6           STRUCTURE UPLOADED

L7           6 SEA SSS SAM L6 (     45 REACTIONS)  
              D SCA  
              D STAT QUE

L8           446 SEA SSS FUL L6 (  4732 REACTIONS)  
              SAVE TEMP L8 JAI943STR6L/A

FILE 'REGISTRY' ENTERED AT 08:30:49 ON 17 OCT 2008

L9           23 SEA ABB=ON PLU=ON L2 AND M/ELS

L10          5 SEA ABB=ON PLU=ON L2 NOT L9  
              D SCA

L11          23 SEA ABB=ON PLU=ON L9 AND X/ELS

## D SCA

FILE 'CASREACT' ENTERED AT 08:32:57 ON 17 OCT 2008  
L12 TRA PLU=ON L8 1- RX : 5601 TERMS

FILE 'REGISTRY' ENTERED AT 08:37:17 ON 17 OCT 2008  
L13 5601 SEA ABB=ON PLU=ON L12/RN  
L14 11 SEA ABB=ON PLU=ON L13 AND L2  
D SCA  
L15 348 SEA ABB=ON PLU=ON L13 AND (M/ELS OR B/ELS OR AS/ELS OR  
TE/ELS OR AT/ELS)  
L16 97 SEA ABB=ON PLU=ON L15 AND X/ELS  
L17 86 SEA ABB=ON PLU=ON L16 NOT L14  
L18 62 SEA ABB=ON PLU=ON L17 AND C/ELS  
L19 24 SEA ABB=ON PLU=ON L17 NOT L18  
D SCA

FILE 'CAPLUS' ENTERED AT 08:45:57 ON 17 OCT 2008  
E LEWIS ACIDS+ALL/CT  
E LEWIS ACIDS+MAX/CT

FILE 'CASREACT' ENTERED AT 08:47:18 ON 17 OCT 2008  
L20 2766 SEA ABB=ON PLU=ON LEWIS ACID?/CW  
L21 9688 SEA ABB=ON PLU=ON LEWIS ACID?/BI,NTE  
L22 7 SEA ABB=ON PLU=ON L8 AND (L20 OR L21)  
D SCA  
L23 134073 SEA ABB=ON PLU=ON L16  
L24 103 SEA ABB=ON PLU=ON L23 (L) L8  
L25 STRUCTURE UPLOADED  
L26 15 SEA SUB=L8 SSS SAM L25 ( 304 REACTIONS)  
L27 331 SEA SUB=L8 SSS FUL L25 ( 3351 REACTIONS)  
L28 66 SEA ABB=ON PLU=ON L27 (L) L23

FILE 'REGISTRY' ENTERED AT 08:57:03 ON 17 OCT 2008  
L29 35 SEA ABB=ON PLU=ON L14 OR L19  
D SCA

FILE 'CASREACT' ENTERED AT 09:01:59 ON 17 OCT 2008  
L30 106670 SEA ABB=ON PLU=ON L29  
L31 15382 SEA ABB=ON PLU=ON L18/CAT  
L32 53 SEA ABB=ON PLU=ON L27 (L) L30  
L33 6 SEA ABB=ON PLU=ON L27 (L) L31  
L34 57 SEA ABB=ON PLU=ON L32 OR L33  
L35 STRUCTURE UPLOADED  
L36 12 SEA SUB=L8 SSS SAM L35 ( 283 REACTIONS)  
L37 239 SEA SUB=L8 SSS FUL L35 ( 2506 REACTIONS)  
L38 42 SEA ABB=ON PLU=ON L37 (L) L30  
L39 5 SEA ABB=ON PLU=ON L37 (L) L31  
L40 45 SEA ABB=ON PLU=ON L38 OR L39  
D SCA

FILE 'STNGUIDE' ENTERED AT 09:19:14 ON 17 OCT 2008

FILE 'CASREACT' ENTERED AT 09:21:09 ON 17 OCT 2008

FILE 'REGISTRY' ENTERED AT 09:24:00 ON 17 OCT 2008  
L41 1 SEA ABB=ON PLU=ON L13 AND NB/ELS  
D SCA  
D RN

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FILE 'CASREACT' ENTERED AT 09:25:01 ON 17 OCT 2008

L42 152 SEA ABB=ON PLU=ON 10026-12-7  
L43 1 SEA ABB=ON PLU=ON L42 (L) L8  
D SCA  
L44 50 SEA ABB=ON PLU=ON L40 OR L22  
D OCC 1- L44  
D COST  
D HIT 30

FILE 'REGISTRY' ENTERED AT 09:35:28 ON 17 OCT 2008

L45 2 SEA ABB=ON PLU=ON L29 AND B/ELS  
D SCA  
L46 1 SEA ABB=ON PLU=ON L45 NOT F/ELS  
L47 1 SEA ABB=ON PLU=ON L45 NOT L46  
D SCA  
D RN

FILE 'CASREACT' ENTERED AT 09:36:56 ON 17 OCT 2008

L\*\*\* DEL 0 S 16872-11-0 R  
L48 2084 SEA ABB=ON PLU=ON 16872-11-0  
L49 1 SEA ABB=ON PLU=ON L48 (L) L38  
L50 0 SEA ABB=ON PLU=ON L48 (L) L39  
L51 49 SEA ABB=ON PLU=ON L44 NOT L49

FILE 'REGISTRY' ENTERED AT 09:37:47 ON 17 OCT 2008

FILE 'CASREACT' ENTERED AT 09:38:15 ON 17 OCT 2008

D OCC L22 1-  
D OCC L38 1-  
D OCC L39 1-  
D OCC 1- L38  
D FHIT L38 3  
D FHIT L38 4  
L52 446 SEA ABB=ON PLU=ON L8/COM  
L53 239 SEA ABB=ON PLU=ON L37/COM  
L54 STRUCTURE UPLOADED  
L55 12 SEA SUB=L8 SSS SAM L54 ( 283 REACTIONS)  
L56 239 SEA SUB=L8 SSS FUL L54 ( 2506 REACTIONS)  
L57 42 SEA ABB=ON PLU=ON L56 (L) L30  
L58 5 SEA ABB=ON PLU=ON L56 (L) L31  
D OCC L57 1-  
D FHIT 5 L38  
D FHIT 6 L38  
D FHIT 7 L38  
D FHIT 17 L38  
D FHIT 21 L38  
L59 STRUCTURE UPLOADED  
L60 9 SEA SUB=L8 SSS SAM L59 ( 136 REACTIONS)  
D SCA  
L61 163 SEA SUB=L8 SSS FUL L59 ( 1426 REACTIONS)  
L62 1 SEA ABB=ON PLU=ON L61 AND L20  
L63 1 SEA ABB=ON PLU=ON L61 AND L21  
L64 30 SEA ABB=ON PLU=ON L61 (L) L30  
L65 2 SEA ABB=ON PLU=ON L61 (L) L31  
L66 30 SEA ABB=ON PLU=ON (L62 OR L63 OR L64 OR L65)  
D OCC 1-  
D COST  
D SCA L65  
D HIT L65 1  
L67 12 SEA ABB=ON PLU=ON L64 AND NS>5

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L68 1 SEA ABB=ON PLU=ON L43 AND L66  
L69 1159 SEA ABB=ON PLU=ON NIOBIUM/BI,CW,NTE  
L70 1 SEA ABB=ON PLU=ON L69 AND L61  
L71 0 SEA ABB=ON PLU=ON L70 AND L49  
L72 1 SEA ABB=ON PLU=ON L70 AND L43

FILE 'CAPLUS' ENTERED AT 10:13:14 ON 17 OCT 2008

L73 643 SEA ABB=ON PLU=ON LOPES C?/AU  
L74 331 SEA ABB=ON PLU=ON LOPES R?/AU  
L75 368 SEA ABB=ON PLU=ON CARDOSO J?/AU  
L76 2399 SEA ABB=ON PLU=ON SILVA J?/AU OR DA SILVA J?/AU OR DASILVA  
J?/AU  
L77 1104 SEA ABB=ON PLU=ON FERREIRA L?/AU  
L\*\*\* DEL 28 S L73 AND L74-L76  
L\*\*\* DEL 22 S L74 AND L75-L78  
L78 28 SEA ABB=ON PLU=ON L73 AND (L74 OR L75 OR L76 OR L77)  
L79 8 SEA ABB=ON PLU=ON L74 AND (L75 OR L76 OR L77)  
L80 2 SEA ABB=ON PLU=ON L75 AND (L76 OR L77)  
L81 16 SEA ABB=ON PLU=ON L76 AND L77  
L82 8 SEA ABB=ON PLU=ON L78 AND (L79 OR L80 OR L81)  
L83 0 SEA ABB=ON PLU=ON L79 AND (L80 OR L81)  
L84 0 SEA ABB=ON PLU=ON L80 AND L81  
L85 8 SEA ABB=ON PLU=ON (L82 OR L83 OR L84)  
L86 446 SEA ABB=ON PLU=ON L8  
L87 3 SEA ABB=ON PLU=ON L86 AND (L73 OR L74 OR L75 OR L76 OR L77)

FILE 'REGISTRY' ENTERED AT 10:17:11 ON 17 OCT 2008

FILE 'CAPLUS' ENTERED AT 10:17:14 ON 17 OCT 2008

D STAT QUE L85  
D STAT QUE L87

FILE 'MEDLINE, EMBASE, BIOSIS, WPIX' ENTERED AT 10:17:32 ON 17 OCT 2008

L88 4 SEA ABB=ON PLU=ON L85

FILE 'ZCAPLUS' ENTERED AT 10:17:43 ON 17 OCT 2008

FILE 'CAPLUS' ENTERED AT 10:17:48 ON 17 OCT 2008

L89 10 SEA ABB=ON PLU=ON L85 OR L87

FILE 'CAPLUS, MEDLINE, EMBASE, WPIX' ENTERED AT 10:18:05 ON 17 OCT 2008

L90 11 DUP REM L89 L88 (3 DUPLICATES REMOVED)  
ANSWERS '1-10' FROM FILE CAPLUS  
ANSWER '11' FROM FILE MEDLINE  
D IBIB ABS L90 1-10  
D IALL L90 11

FILE 'REGISTRY' ENTERED AT 10:18:43 ON 17 OCT 2008

FILE 'CASREACT' ENTERED AT 10:18:46 ON 17 OCT 2008

D STAT QUE L43  
D IBIB ABS HIT L43 1

FILE 'REGISTRY' ENTERED AT 10:19:27 ON 17 OCT 2008

FILE 'CASREACT' ENTERED AT 10:19:29 ON 17 OCT 2008

D STAT QUE L62  
D STAT QUE L63  
D STAT QUE L64  
D STAT QUE L65



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L91            30 SEA ABB=ON   PLU=ON   L62 OR L63 OR L64 OR L65  
              D IBIB ABS HIT L91 1-30

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES:    15 OCT 2008    HIGHEST RN 1061881-29-5

DICTIONARY FILE UPDATES:   15 OCT 2008    HIGHEST RN 1061881-29-5

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

FILE ZCAPLUS

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FILE COVERS 1907 - 17 Oct 2008   VOL 149 ISS 17

FILE LAST UPDATED: 16 Oct 2008   (20081016/ED)

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FILE CONTENT:1840 - 12 Oct 2008 VOL 149 ISS 16

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FILE STNGUIDE  
FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: Oct 10, 2008 (20081010/UP).

FILE MEDLINE  
FILE LAST UPDATED: 16 Oct 2008 (20081016/UP). FILE COVERS 1949 TO DATE.

MEDLINE has been updated with the National Library of Medicine's revised 2008 MeSH terms. See HELP RLOAD for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

See HELP RANGE before carrying out any RANGE search.

MEDLINE Accession Numbers (ANs) for records from 1950-1977 have been converted from 8 to 10 digits. Searches using an 8 or 10 digit AN will retrieve the same record. The 10-digit ANs can be expanded, searched, and displayed in all records from 1949 to the present.

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FILE EMBASE

FILE COVERS 1974 TO 17 Oct 2008 (20081017/ED)

EMBASE was reloaded on March 30, 2008.

EMBASE is now updated daily. SDI frequency remains weekly (default) and biweekly.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Beginning January 2008, Elsevier will no longer provide EMTREE codes as part of the EMTREE thesaurus in EMBASE. Please update your current-awareness alerts (SDIs) if they contain EMTREE codes.

For further assistance, please contact your local helpdesk.

FILE BIOSIS

FILE COVERS 1926 TO DATE.

CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT FROM JANUARY 1926 TO DATE.

RECORDS LAST ADDED: 15 October 2008 (20081015/ED)

BIOSIS has been augmented with 1.8 million archival records from 1926 through 1968. These records have been re-indexed to match current BIOSIS indexing.

FILE WPIX

FILE LAST UPDATED: 13 OCT 2008 <20081013/UP>

MOST RECENT UPDATE: 200865 <200865/DW>

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>>> IPC Reform backfile reclassifications have been loaded to the end of June 2008. No update date (UP) has been created for the reclassified documents, but they can be identified by 20060101/UPIC and 20061231/UPIC, 20070601/UPIC, 20071001/UPIC, 20071130/UPIC, 20080401/UPIC and 20080701/UPIC. ECLA reclassifications to June and US national classifications to the end of April 2008 have also been loaded. Update dates 20080401 and 20080701/UPEC and /UPNC have been assigned to these. <<<

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FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE

<http://scientific.thomsonreuters.com/support/patents/coverage/latestupdate>

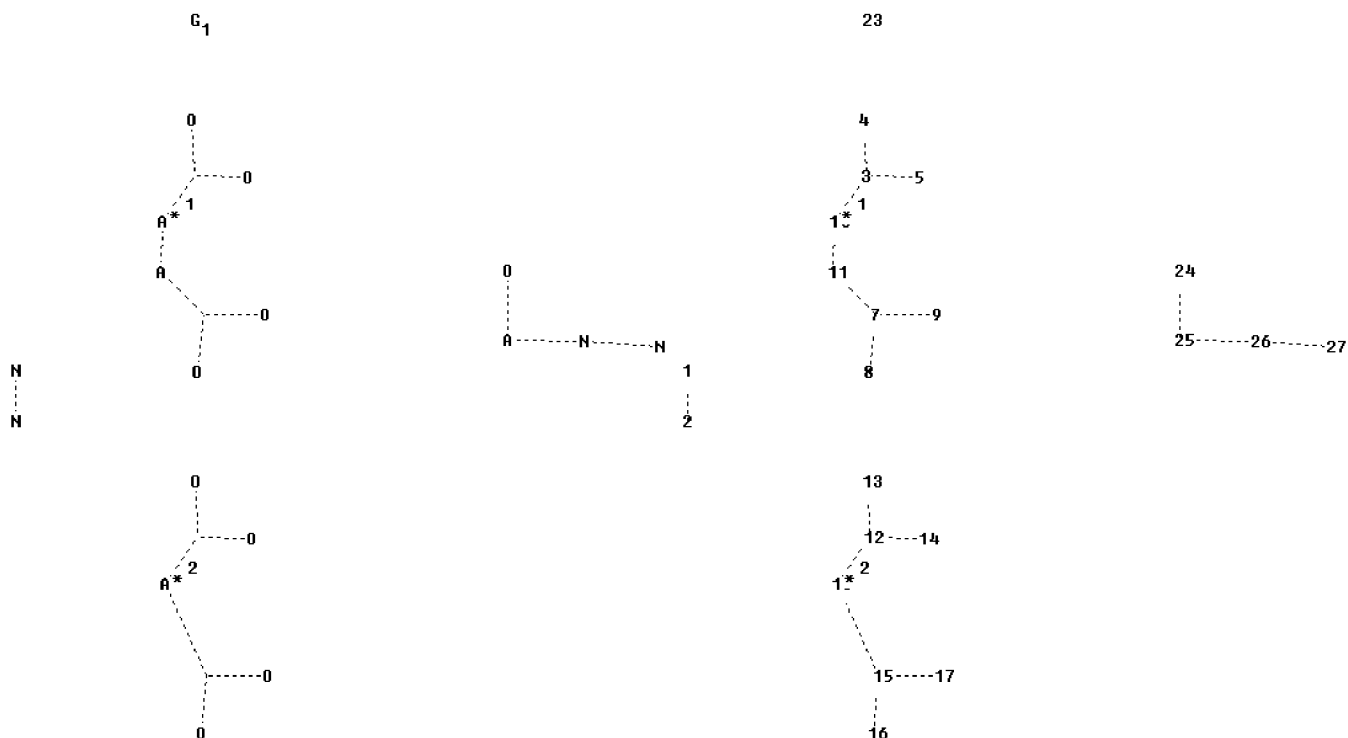
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[http://www.stn-international.com/archive/presentations/DWPIAnaVist2\\_0608.p](http://www.stn-international.com/archive/presentations/DWPIAnaVist2_0608.p)

>>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

Uploading L6.str

10/595943



```
chain nodes :
3 4 5 7 8 9 12 13 14 15 16 17 23 24
ring/chain nodes :
1 2 10 11 18 25 26 27
chain bonds :
3-4 3-5 3-10 7-8 7-9 7-11 12-13 12-14 12-18 15-16 15-17 15-18 24-25

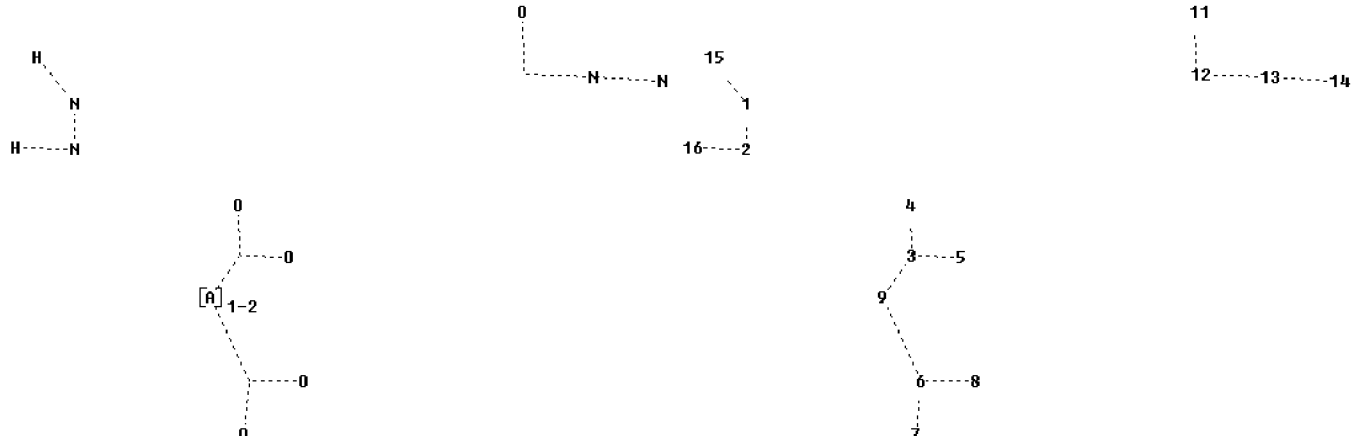
ring/chain bonds :
1-2 10-11 25-26 26-27
exact/norm bonds :
1-2 3-4 3-5 3-10 7-8 7-9 7-11 10-11 12-13 12-14 12-18 15-16 15-17 15-18
24-25 25-26 26-27
```

G1:[\*1],[\*2]

```
Connectivity :
3:3 E exact RC ring/chain 4:1 E exact RC ring/chain 5:1 E exact RC ring/chain
7:3 E exact RC ring/chain 8:1 E exact RC ring/chain 9:1 E exact RC ring/chain
12:3 E exact RC ring/chain
13:1 E exact RC ring/chain 14:1 E exact RC ring/chain 15:3 E exact RC ring/chain
16:1
E exact RC ring/chain 17:1 E exact RC ring/chain 24:1 E exact RC ring/chain
Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
23:CLASS 24:CLASS
25:CLASS 26:CLASS 27:CLASS
fragments assigned product role:
containing 24
fragments assigned reactant/reagent role:
containing 1
containing 23
```

10/595943

Uploading L59.str



```
chain nodes :
4 5 7 8 11 15 16
ring/chain nodes :
1 2 3 6 9 12 13 14
chain bonds :
1-15 2-16 3-4 3-5 6-7 6-8 11-12
ring/chain bonds :
1-2 3-9 6-9 12-13 13-14
exact/norm bonds :
1-2 1-15 2-16 3-4 3-5 3-9 6-7 6-8 6-9 11-12 12-13 13-14
```

```
Connectivity :
3:3 E exact RC ring/chain 4:1 E exact RC ring/chain 5:1 E exact RC ring/chain
6:3 E exact RC ring/chain 7:1 E exact RC ring/chain 8:1 E exact RC ring/chain
11:1 E exact RC ring/chain
```

```
Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS
fragments assigned reactant role:
containing 3
fragments assigned product role:
containing 11
fragments assigned reactant/reagent role:
containing 1
reaction site bonds:
12-13:CC
node mappings:
3:12 1:13
```

=>